

SPHERE PACKINGS IV

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1. INTRODUCTION AND REVIEW

1.1. The steps. The Kepler conjecture asserts that no packing of spheres in three dimensions has density greater than $\pi/\sqrt{18} \approx 0.74048$. This paper is one of a series of papers devoted to the Kepler conjecture. This series began with [I], which proposed a line of research to prove the conjecture, and broke the conjecture into smaller conjectural steps which imply the Kepler conjecture. The steps were intended to be equal in difficulty, although some have emerged as more difficult than others. This paper completes part of the fourth step. The main result is Theorem 4.4.

As a continuation of [F] and [III], this paper assumes considerable familiarity with the constructions, terminology, and notation from these earlier papers. See [F] for the definitions of quasi-regular tetrahedra, upright and flat quarters and their diagonals, anchors, Rogers simplices, standard clusters, standard regions, the Q -system, V -cells, local V -cells, and decomposition stars.

We will use a number of constants and functions from [I] and [F]: $\delta_{oct} = (\pi - 2\zeta^{-1})/\sqrt{8}$, $pt = -\pi/3 + 2\zeta^{-1}$, $\zeta^{-1} = 2 \arctan(\sqrt{2}/5)$, $t_0 = 1.255$, $\phi(h, t)$, $\phi_0 = \phi(t_0, t_0)$, $\Gamma(S)$ is the compression, $\text{vor}(S)$ is the analytic Voronoi function, $\text{vor}(\cdot, t)$ and $\text{vor}_0 = \text{vor}(\cdot, t_0)$ are the truncated Voronoi functions, $\sigma(S)$ is the score, $\tau(S)$ measures what is squandered by a simplex, $\text{dih}(S)$ is the dihedral angle along the first edge of a simplex, sol is the solid angle, $R(a, b, c)$ is a Rogers simplex with parameters $a \leq b \leq c$, and $S(y_1, \dots, y_6)$ is a simplex with edge lengths y_i with the standard conventions from [I] on the ordering of edges. The definitions of $\sigma(S)$ and $\tau(S)$ are particularly involved. The definition depends on the structure and *context* of S [F.3].

At the heart of this approach is a geometric structure, called the *decomposition star*, constructed around the center of each sphere in the packing. A function σ , called the *score*, is defined on the space of all decomposition stars. An upper bound of $8pt \approx 0.4429$ on the score implies the Kepler conjecture [F, Proposition 3.14]. A second function τ , measuring what is *squandered*, is defined on the space of decomposition stars. If a decomposition star squanders more than $(4\pi\zeta - 8)pt \approx 14.8pt \approx 0.819$, then it scores less than $8pt$.

1.2 Exceptional regions.

A standard region is said to be *exceptional* if it is not a triangle or quadrilateral. The vertices of the packing of height at most 2.51 that are contained in the closed cone over the standard region are called its *corners*.

The results of this paper are based on a number of inequalities listed in the appendix. These inequalities are grouped into collections denoted \mathbf{A}_i .

1.3 Organization of this paper.

Lemmas, Remarks, Propositions, and so forth, are numbered according to the following conventions. The paper is divided into five sections and Appendices. Each section is divided into a number of subsections. The reference $n.m$ refers to Subsection m of Section n , or more briefly, Section $n.m$. For instance, this is Section 1.3. In general, lemmas, remarks, and so forth, are numbered according to the subsection in which they appear. Thus, Proposition 3.7 is the unique Proposition in Section 3.7. When more than one Lemma appears in a subsection, they are numbered consecutively. Thus, the three lemmas of Section 3.8 are Lemmas 3.8.1, 3.8.2, and 3.8.3.

Appendix 1 contains long listings of inequalities that are used throughout the paper. These inequalities are grouped into 24 sections $\mathbf{A}_1, \dots, \mathbf{A}_{24}$. Each inequality is labeled with an integer $1, \dots, k$ and a unique nine-digit identification number. In the body of the paper, each inequality is identified by its Section and integer label. Thus, Inequality $\mathbf{A}_8.4$ is the fourth inequality in Section \mathbf{A}_8 of Appendix 1. The nine-digit identification code is used to identify the inequality in the archive of computer code that was used to test and prove the inequality. These numeric codes make it easy to locate computer files that deal with a particular inequality.

2. THE FINE DECOMPOSITION

2.1. Overview of the Fine Decomposition.

In Section 2, we define a decomposition of each local V -cell V_P , called the *fine decomposition* of V_P . Let V be the V -cell at the origin. Let P be an exceptional cluster. Recall that the part of V in the cone $C(P)$ over P is called the local V -cell V_P . Let $V_P(t_0)$ be the intersection of V_P with the ball $B(t_0)$ of radius $t_0 = 1.255$. We write V_P as the disjoint union of $V_P(t_0)$ and its complement δ_P .

Let v be an enclosed vertex of height between 2.51 and $2\sqrt{2}$. Assume that there is an upright quarter in the Q -system with diagonal $(0, v)$. We call $(0, v)$ an *upright diagonal*. We will define $\delta_P(v) \subset \delta_P$. It will be a subset of a set of the form $C(D_v) \cap \delta_P$ for some subset D_v of the unit sphere. The sets D_v will be defined so as not to overlap one another for distinct v . Then the sets $\delta_P(v)$ do not overlap one another either. We will give an explicit formula for the volume of $\delta_P(v)$.

We will define a set \mathcal{S} of simplices in $C(V_P)$. The vertices of the simplices will be vertices of the packing, and their edges will have length at most $2\sqrt{2}$. The sets $C(S)$, for distinct $S \in \mathcal{S}$, will not overlap. Over a simplex $S \in \mathcal{S}$, the local V -cell will be truncated at a radius $t_S \geq t_0$. After defining the constants t_S , we will set

$$V_S(t_S) = C(S) \cap B(t_S) \cap V_P.$$

If $V_P \cap C(S) \subset B(t_S) \subset B(t'_S)$, then $V_S(t_S) = V_S(t'_S)$.

Since $t_S \geq t_0$, the sets $V_S(t_S)$ and δ_P may overlap. Nevertheless, we will show that $V_S(t_S)$ does not overlap any $\delta_P(v)$. Let $\tilde{V}_P(t_0)$ be the set of points in $V_P(t_0)$

that do not lie in $C(S)$, $S \in \mathcal{S}$. We will derive an explicit formula for the volume and score of $\tilde{V}_P(t_0)$.

In V_P , there are nonoverlapping sets

$$\delta_P(v), \quad V_S(t_S), \quad \tilde{V}_P(t_0).$$

Let δ'_P be the complement in V_P of the union of these sets. These sets give a decomposition of V_P , called the fine decomposition of the local V -cell V_P . Corresponding to the fine decomposition is a formula for the score V_P of the form

$$\sigma(V_P) = \sigma(\tilde{V}_P(t_0)) + \sum_S \sigma(V_S(t_S)) - \sum_v 4\delta_{oct} \text{vol}(\delta_P(v)) - 4\delta_{oct} \text{vol}(\delta'_P).$$

Since $\text{vol}(\delta'_P) \geq 0$, we obtain an upper bound on the score of V_P by dropping the rightmost term.

2.2. V -cells.

Let \mathcal{Q}_0 be the set of simplices in the Q -system with a vertex at the origin. If x lies in the Voronoi cell at the origin, but not in the V -cell, then either x belongs to a simplex in \mathcal{Q}_0 or x belongs to the protruding tip from a simplex in \mathcal{Q}_0 . In either case, $x \in C(S)$, for some $S \in \mathcal{Q}_0$. Consequently, the part of the Voronoi cell over the complement of $C(S)$, for all $S \in \mathcal{Q}_0$, is contained in the V -cell.

2.3. The set $\delta_P(v)$.

Let $(0, v)$ be the diagonal of an upright quarter in \mathcal{Q}_0 and in the cone over P . We define $\delta_P(v) \subset C(D_v) \cap \delta_P$ for an appropriate subset D_v of the unit sphere.

Let D_0 be the spherical cap on the unit sphere, centered along $(0, v)$ and having arcradius θ , where $\cos \theta = |v|/(2\eta_0(|v|/2))$, and $\eta_0(h) = \eta(2h, 2, 2.51)$. The area of D_0 is $2\pi(1 - \cos \theta)$. Let v_1, \dots, v_k be the anchors around $(0, v)$ indexed cyclically. The projections of the edges (v, v_i) (extended as necessary) slice the spherical cap into k wedges W_i , between (v, v_i) and (v, v_j) , where $j \equiv i + 1 \pmod k$, so that $D_0 = \cup W_i$.

Let \mathcal{W} be the set of wedges $W = W_i$ such that either

- (1) W occupies more than half the spherical cap (so that its area is at least $\pi(1 - \cos \theta)$), or
- (2) $|v_i - v_j| \geq 2.77$, $\text{rad}(0, v, v_i, v_j) > \eta_0(|v|/2)$, and the circumradius of $(0, v_i, v_j)$ or (v, v_i, v_j) is $\geq \sqrt{2}$.

Fix i, j , with $j \equiv i + 1 \pmod k$. If $W = W_i$ is a wedge in \mathcal{W} , let $(0, v_i, v)^\perp$ be the plane through the origin and the circumcenter of $(0, v_i, v)$, perpendicular to $(0, v_i, v)$. Skip the following step if the circumradius of $(0, v_i, v)$ is greater than $\eta_0(|v|/2)$, but if the circumradius is at most this bound, let c_i be the intersection of $(0, v_i, v)^\perp$ with the circular boundary of W . Extend W by adding to W the spherical triangle with vertices the projections of v, v_i , and c_i . Similarly, extend W with the triangle from (v, v_j, c_j) , if the circumradius of $(0, v_j, v)$ permits. (An example of this is illustrated in F.4.6.) Let W^e be extension of the wedge obtained by adding these two spherical triangles.

We will define $\delta_P(W^e) \subset C(W^e) \cap \delta_P$. Then $\delta_P(v)$ is defined as the union of $\delta_P(W^e)$, for $W \in \mathcal{W}$. Let

$$E_w = \{x : 2x \cdot w \leq w \cdot w\},$$

for $w = v, v_i, v_j$. These are half-spaces bounding the Voronoi cell. Set $E_\ell = E_{v_\ell}$.

If (2) holds, we let c be the projection of the circumradius of $(0, v_i, v_j, v)$ to the unit sphere. The arclength from c to the projection of v is θ' , where

$$\cos \theta' = |v|/(2 \text{ rad}) < |v|/(2\eta_0) = \cos \theta.$$

We conclude that $\theta' > \theta$ and c does not lie in D_0 .

In both cases (1) and (2) set

$$\delta_P(W^e) = (E_v \cap E_i \cap E_j \cap C(W^e)) \setminus B(t_0).$$

Observe that

$$E_v \cap E_i \cap E_j \cap C(W^e)$$

is the union of four Rogers simplices

$$R(|w|/2, \eta(0, v, v_\ell), \eta_0(|v|/2)), \quad w = v, v_\ell, \quad \ell = i, j$$

and a conic wedge over W between c_i and c_j . (The inequality $\theta' > \theta$ implies that the Rogers simplices do not overlap.)

Lemma. $\delta_P(W^e) \subset V_P$.

Proof. First assume for a contradiction that some part of the wedge between c_i and c_j overlaps the V -cell at some other vertex v' . This forces $\eta(0, v, v') < \eta_0(|v|/2)$, and v' must then be an anchor. But for anchors, the separation of V -cells has been achieved by the half-spaces E_* .

Now suppose one of the Rogers simplices along $(0, v, v_i)$ overlaps the V -cell at some vertex v' . If v' lies on the opposite side of the plane $(0, v, v_i)$ from W^e , then in order to meet, the face $(0, v, v_i)$ of $(0, v, v_i, v')$ must have negative orientation. This forces $(0, v, v_i, v')$ to be a quarter [F]. It is in the Q -system because one and hence all quarters along $(0, v)$ lie in the Q -system. Thus any protruding tip from v' is reapportioned among neighboring V -cells, so that such a point of $\delta_P(W^e)$ lies in the V -cell.

Take v' and W^e to lie on the same side of $(0, v, v_i)$. To overlap, the circumradius of $(0, v, v_i, v)$ must be less than $\eta_0(|v|/2)$. Then $\eta(0, v, v') < \eta_0(|v|/2)$, forcing v' to be an anchor. Since v_i and v_j are chosen to be consecutive, we find that $v' = v_j$. But then the condition (2) gives the contradiction $\text{rad}(0, v, v_i, v') \geq \eta_0(|v|/2)$. \square

2.4. Overlap.

Proposition. *The sets $\delta_P(W^e)$ do not overlap.*

Proof. This is clear for two sets around the same vertex v . In general, this follows from the fact that the sets W^e do not overlap on the unit sphere. We use the faces of the V -cell to separate them. In the notation of Sections 2.1-2.3, the part of the wedge W between c_i and c_j lies under the face of the V -cell associated with v , the vertex used to construct W . Hence, these pieces do not overlap at different vertices. Similarly, two of the Rogers simplices lie under the face of the V -cell associated with v . The remaining two Rogers simplices lie under the faces of V -cells of two of the anchors of v . A vertex v_i may be the anchor of more than one upright diagonal $(0, v)$ and $(0, v')$. Nevertheless, the corresponding Rogers simplices do not overlap

because each Rogers simplex for W^e at v will lie under the triangular part of the face determined by $v_i/2$ and the edge of the V -face dual to the triangle $(0, v_i, v)$, and the Rogers simplex for W'^e at v' will lie under a corresponding triangular part of the face. These triangles do not overlap, so the extended wedges cannot either. \square

Suppose that the faces of the V -cell dual to two vertices v_1 and v_2 (of height at most $2\sqrt{2}$) share an edge. On the face dual to v_1 , we take the triangle formed by $v_1/2$ and the common edge, and call it the (v_1, v_2) -triangle. (Since $|v_1| \leq 2\sqrt{2}$, $v_1/2$ lies on the face dual to v_1 .) The proof shows that the set $\delta_P(v)$ lies under the face dual to v or under the (v_i, v) -triangles of anchors v_i of v .

2.5. Some simplices.

We consider three types of simplices S_A, S_B, S_C . Each type has its vertices at vertices of the packing. The edge lengths of these simplices are at most $2\sqrt{2}$.

S_A . This family consists of simplices $S(y_1, \dots, y_6)$ whose edge lengths satisfy

$$y_1, y_2, y_3 \in [2, 2.51], \quad y_4, y_5 \in [2.51, 2.77], \quad y_6 \in [2, 2.51], \quad \text{and } \eta(y_4, y_5, y_6) < \sqrt{2}.$$

(These conditions imply $y_4, y_5 < 2.697$, because $\eta(2.697, 2.51, 2) > \sqrt{2}$.)

S_B . This family consists of certain flat quarters that are part of an isolated pair of flat quarters. It consists of those satisfying $y_2, y_3 \leq 2.23, y_4 \in [2.51, 2\sqrt{2}]$.

S_C . This family consists of certain simplices $S(y_1, \dots, y_6)$ with edge lengths satisfying $y_1, y_4 \in [2.51, 2\sqrt{2}], y_2, y_3, y_5, y_6 \in [2, 2.51]$. We impose the condition that the first edge is the diagonal of some upright quarter in the Q -system, and that the upper endpoints of the second and third edges (that is, the second and third vertices of the simplex) are consecutive anchors of this diagonal. We also assume that $y_4 \leq 2.77$, or that both face circumradii of S along the fourth edge are at most $\sqrt{2}$.

Lemma. *If a vertex w is enclosed over a simplex S of type S_A, S_B , or S_C , then its height is greater than 2.77. Also, $(0, w)$ is not the diagonal of an upright quarter in the Q -system.*

Proof. In case S_A , $\eta(y_4, y_5, y_6) < \sqrt{2}$, so an enclosed vertex must have height greater than $2\sqrt{2}$. It is too long to be the diagonal of a quarter.

In case S_B , we use the fact that the isolated quarter does not overlap any quarter in the Q -system. We recall that a function \mathcal{E} , defined in [F], measures the distance between opposing vertices in a pair of simplices sharing a face. An enclosed vertex has length at least

$$\mathcal{E}(S(2, 2, 2, 2\sqrt{2}, 2.51, 2.51), 2.51, 2, 2) > 2.77.$$

By the symmetry of isolated quarters, this means that the diagonal of a flat quarter must also be at least 2.77.

In case S_C , the same calculation gives that the enclosed vertex w has height at least 2.77. Let the simplex S be given by $(0, v, v_1, v_2)$, where $(0, v)$ is the upright diagonal. By Lemma F.1.5, v_1 and v_2 are anchors of $(0, w)$. The edge between w and its anchor cannot cross (v, v_i) by Lemma F.1.3. (Recall that two sets are said to *cross* if their projections overlap.) The distance between w and v is at most 2.51 by Lemma F.1.9. If $(0, w)$ is the diagonal of an upright quarter, the quarter takes the form $(0, w, v_1, v_3)$, or $(0, w, v_2, v_3)$ for some v_3 , by Lemma F.1.8. If both

of these are quarters, then the diagonal (v_1, v_2) has four anchors v , w , 0 , and v_3 . The selection rules for the Q -system place the quarters around this diagonal in the Q -system. So neither $(0, w, v_1, v_3)$ nor $(0, w, v_2, v_3)$ is in the Q -system. Suppose that $(0, w, v_1, v_3)$ is a quarter, but that $(0, w, v_2, v_3)$ is not. Then $(0, w, v_1, v_3)$ forms an isolated pair with (v_1, v_2, v, w) . In either case the quarters along $(0, w)$ are not in the Q -system. \square

Remark. *The proof of this lemma does not make use of all the hypotheses on S_C . The conclusion holds for any simplex $S(y_1, \dots, y_6)$, with $y_1, y_4 \in [2.51, 2\sqrt{2}]$, $y_2, y_3, y_5, y_6 \in [2, 2.51]$.*

2.6. Disjointness.

Let $S = (0, v_1, v_2, v_3)$ be a simplex of type S_A , S_B , or S_C . An edge (v_4, v_5) of length at most $2\sqrt{2}$ such that $|v_4|, |v_5| \leq 2.51$ cannot cross two of the edges (v_i, v_j) of S . In fact, it cannot cross any edge (v_i, v_j) with $|v_i|, |v_j| \leq 2.51$ by Lemma F.1.6. The only possibility is that the edge (v_4, v_5) crosses the two edges with endpoint v_1 , with $|v_1| \geq 2.51$ in case S_C . But this too is impossible by Lemma F.1.8.

Similar arguments show that the same conclusion holds for an edge (v_4, v_5) of length at most 2.51 such that $|v_4| \leq 2.51$, $v_5 \leq 2\sqrt{2}$. The only additional fact that is needed is that (v_4, v_5) cannot cross the edge between the vertex v of an upright diagonal $(0, v)$ and an anchor [F.1.3].

Now take two simplices S , S' , each of type S_A , S_B , S_C , or a quarter in the Q -system.

Lemma. *S and S' do not overlap.*

Proof. We remark that we are tacitly assuming that the standard region is exceptional, and we exclude the case of conflicting diagonals in a quad cluster. We claim that no vertex w of S is enclosed over S' . Otherwise, w must have height at least 2.51, so that $(0, w)$ is the diagonal of an upright in the Q -system, and this is contrary to Lemma 2.5. Similarly, no vertex of S' is enclosed over S .

Let (v_1, v_2) be an edge of S crossing an edge (v_3, v_4) of S' . By the preceding remarks, neither of these edges can cross two edges of the other simplex. The endpoints of the edges are not enclosed over the other simplex. This means that one endpoint of each edge (v_1, v_2) and (v_3, v_4) is a vertex of the other simplex. This forces S and S' to have three vertices in common, say 0 , v_2 , and v_3 . We have $S = (0, v_1, v_3, v_2)$ and $S' = (0, v_3, v_2, v_4)$. If $|v_2| \in [2.51, 2\sqrt{2}]$, then we see that the anchors v_3, v_4 of $(0, v_2)$ are not consecutive. This is impossible for simplices of type S_C and upright quarters. Thus, v_2 and v_3 have height at most 2.51. We conclude, without loss of generality, that $|v_4| \in [2.51, 2\sqrt{2}]$ and $|v_1 - v_2| \geq 2.51$ [F.1].

The heights of the vertices of S are at most 2.51, so it has type S_A or S_B , or it is a flat quarter in the Q -system. If S' is an upright quarter in the Q -system, then it does not overlap an isolated quarter or a flat quarter in the Q -system, so S has type S_A . This imposes the contradictory constraints on S_A

$$2.77 \geq |v_1 - v_2| \geq \mathcal{E}(S(2.51, 2, 2, 2\sqrt{2}, 2.51, 2.51), 2, 2, 2) > 2.77.$$

Thus S' has type S_C . This forces S to have type S_A . We reach the same contradiction $2.77 \geq \mathcal{E} > 2.77$. \square

2.7 Separation of simplices of type S_A .

Let $V_S = V_P \cap C(S)$, for a simplex S of type S_A , S_B , or S_C . We truncate V_S to $V_S(t_S)$ by intersecting V_S with a ball of radius t_S . The parameters t_S depend on S .

If S has type S_A , we use $t_S = +\infty$ (no truncation). If v is enclosed over $S = (0, v_1, v_2, v_3)$, then since $\eta(v_1, v_2, v_3) < \sqrt{2}$, the face (v_1, v_2, v_3) has positive orientation for S and (v, v_1, v_2, v_3) . This implies that the V -cells at v and 0 do not intersect, and there is no need to truncate. If a simplex adjacent to S has negative orientation along a face shared with S_A , then it must be a quarter $Q = (0, v_4, v_1, v_2)$ [F.2.2] or quasi-regular tetrahedron. It cannot be an isolated quarter because of the edge length constraint 2.77 on simplices of type S_A . If it is in the Q -system, it does not interfere with the V -cell over S . Assume that it is not in the Q -system. There must be a conflicting diagonal $(0, w)$, where w is enclosed over Q . (w cannot be enclosed over S by results of Lemma 2.6.) This shields the V -cell at v_4 from $C(S)$ by the two faces $(0, w, v_1)$ and $(0, w, v_2)$ of quarters in the Q -system.

This shows that nothing external to a simplex of type S_A affects the shape of $V_S(t_S)$, so that $V_S(t_S)$ can be computed from S alone. Similarly, $V_S(t_S)$ does not influence the external geometry, since all faces have positive orientation.

We also remark that $V_S(t_S)$ does not overlap any of the sets $\delta_P(v)$. This is evident because the two types of sets lie under the faces of V -cells associated with different vertices of the packing. A set $\delta_P(v)$ lies under the face of the V -cell dual to v or under the (w, v) -triangles of anchors w of V . But $V_S(t_S)$ lies under the (v_i, v_j) -triangles, for the edges (v_i, v_j) of S . (See Section 2.4.)

Our justification that $V_S(t_S)$ can be treated as an independently scored entity is now complete.

2.8. Separation of simplices of type S_B .

If $S(y_1, \dots, y_6)$ has type S_B , we label vertices so that the diagonal is the fourth edge, with length y_4 . We set $t_S = 1.385$. The calculation of \mathcal{E} in Section 2.5 shows that any enclosed vertex over S has height at least $2.77 = 2t_S$.

Vertices outside $C(S)$ cannot affect the shape of $V_S(t_S)$. In fact, such a vertex v' would have to form a quarter or quasi-regular tetrahedron with a face of S . The V -cell at v' cannot meet $C(S)$ unless it is a quarter that is not in the Q -system. But by definition, an isolated quarter is not adjacent (along a face along the diagonal) to any other quarters.

To separate the scoring of $V_S(t_S)$ from the rest of the standard cluster, we also show that the terms of Formula F.3.5 for $V_S(t_S)$ lie in the cone $C(S)$. This is more than a formality because S can have negative orientation along the face F formed by the origin and the diagonal (the fourth edge).

Let $\arccos(a, b, c) = \arccos((a^2 + b^2 - c^2)/(2ab))$ be the angle opposite the edge of length c in a triangle with sides a, b, c . Let $\beta_\psi(y_1, y_3, y_5) \in [0, \pi/2]$ be defined by the equations

$$\begin{aligned} \cos^2 \beta_\psi &= (\cos^2 \psi - \cos^2 \theta) / (1 - \cos^2 \theta), \text{ for } \psi \leq \theta, \\ \theta &= \arccos(y_1, y_3, y_5). \end{aligned}$$

If we form a triangle $(0, v_1, v_3)$, where $|v_1| = y_1$, $|v_3| = y_3$, $|v_1 - v_3| = y_5$, then θ is the angle at the origin between v_1 and v_3 . If we place a spherical cap of arcradius ψ on the unit sphere centered along $(0, v_1)$, then the angle along $(0, v_3)$ between the

plane $(0, v_1, v_3)$ and the plane tangent to the spherical cap passing through $(0, v_3)$ is $\beta_\psi(y_1, y_3, y_5)$.

Let $S = (0, v_1, v_2, v_3)$, where v_i is the endpoint of the i th edge. We establish that the conic and Rogers terms of Formula F.3.5 lie over $C(S)$ by showing that $\beta_\psi(y_1, y_3, y_5) < \text{dih}_3(S(y_1, \dots, y_6))$, where dih_3 is the dihedral angle along the third edge. We use $\cos \psi = y_1/2.77$ and assume $y_2, y_3 \in [2, 2.23]$. See **A**₁.

The reasons given in Section 2.7 for the disjointness of $\delta_P(v)$ and $V_S(t_S)$ apply to simplices of type S_B as well. This completes the justification that $V_S(t_S)$ is an object that can be treated in separation from the rest of the local V -cell.

2.9. Separation of simplices of type S_C .

If $S(y_1, \dots, y_6)$ is of type S_C , we label vertices so that the upright diagonal is the first edge. We use $t_S = +\infty$ (no truncation). Each face of S has positive orientation by F.2.2. So $V_S(t_S) \subset S$.

Vertices outside S cannot affect the shape of $V_S(t_S)$. Any vertex v' would have to form a quarter along a face of S . If the shared face lies along the first edge, it is a quarter Q in the Q -system, because one and hence all quarters along this edge are in the Q -system. If the shared face lies along the fourth edge, then its length is at most 2.77, so that the quarter cannot be part of an isolated pair. If it is not in the Q -system, there must be a conflicting diagonal. The two faces along this conflicting diagonal of the adjacent pair in the Q -system (that is, the pair taking precedence over Q in the Q -system) shield the V -cell at v' from S .

The reasons given in Section 2.7 for the disjointness of $\delta_P(v)$ and $V_S(t_S)$ apply to simplices of type S_C as well. This completes the justification that $V_S(t_S)$ is an object that can be treated in separation from the rest of the local V -cell.

2.10. Simplices of type S'_C .

We introduce a small variation on simplices of type S_C , called type S'_C . We define a simplex $(0, v, v_1, v_2)$ of type S'_C to be one satisfying the following conditions. (1) The edge $(0, v)$ is an upright diagonal of an upright quarter in the Q -system. (2) $|v_2| \in [2.45, 2.51]$. (3) $|v - v_2| \in [2.45, 2.51]$. (4) The edge (v_1, v_2) is a diagonal of a flat quarter with face $(0, v_1, v_2)$.

On simplices S of type S'_C , we label vertices so that the upright diagonal is the first edge. We use $t_S = +\infty$ (no truncation). Each face of S has positive orientation by F.2.2. So $V_S(t_S) \subset S$.

Simplices of type S'_C are separated from quarters in the Q -system and simplices of types S_A and S_B by procedures similar to those described for type S_C . The following lemma is helpful in this regard.

Lemma. *The flat quarter along the face $(0, v_1, v_2)$ is in the Q -system.*

Proof.

$$\mathcal{E}(S(2, 2, 2.45, 2\sqrt{2}, 2t_0, 2t_0), 2, 2, 2) > 2\sqrt{2},$$

so nothing is enclosed over the flat quarter.

$$\mathcal{E}(S(2, 2, 2, 2\sqrt{2}, 2t_0, 2t_0), 2t_0, 2.45, 2) > 2\sqrt{2},$$

so no edge between vertices of the packing can cross inside the anchored simplex. This implies that the flat quarter does not have a conflicting diagonal and is not part of an isolated pair. \square

Similar arguments show that there is not a simplex with negative orientation along the top face of S .

2.11. Scoring.

The construction of the fine decomposition of the local V -cell V_P is now complete. It consists of the pieces

- $\delta_P(v)$, for each diagonal $(0, v)$ of an upright quarter in the Q -system,
- truncations of Voronoi pieces $V_S(t_S)$ for simplices of type S_A , S_B , or S_C (S'_C), over $C(P)$,
- $\tilde{V}_P(t_0)$, the truncation at t_0 of all parts of V_P that do not lie in any of the cones $C(S)$ over simplices of type S_A , S_B or S_C ,
- δ'_P , the part not lying in any of the preceding.

By the results of Sections 2.7–2.9, the score of V_P can be broken into a corresponding sum,

$$\begin{aligned}\sigma(P) &= \sum_Q \sigma(Q) + \sigma(V_P), \text{ for quarters } Q \text{ in the } Q\text{-system,} \\ \sigma(U) &= 4(-\delta_{oct}\text{vol}(U) + \text{sol}(U)/3), \quad \text{where } U = V_P, V_S(t_S), \tilde{V}_P(t_0), \\ \sigma(V_P) &= \sigma(\tilde{V}_P(t_0)) + \sum_{S_A, S_B, S_C} \sigma(V_S(t_S)) - \sum_v 4\delta_{oct}\text{vol}(\delta_P(v)) - 4\delta_{oct}\text{vol}(\delta'_P).\end{aligned}$$

By dropping the final term, $4\delta_{oct}\text{vol}(\delta'_P)$, we obtain an upper bound on $\sigma(V_P)$. Because of the separation results of Sections 2.7–2.9, we may score $\tilde{V}_P(t_0)$ by the Formula F.3.7. Bounds on the score of simplices of type S_B appear in **A**₁.

3. UPRIGHT QUARTERS

3.1. Definitions.

Fix an exceptional cluster R . Throughout this paper, we assume that R lies on a star of score at least $8pt$. It is to be understood, when we say that a standard region does not exist, that we mean that there exists no such region on any star scoring more than $8pt$.

In Section 3, we discuss how to eliminate many cases of upright diagonals. The results are summarized at the end of the section (3.10).

If R is a standard cluster or region, we write $V_R(t)$ for the intersection of the local V -cell V_R with a ball $B(t)$, centered at the origin, of radius t . We generally take $t = t_0 = 1.255 = 2.51/2$. If $(0, v)$, of length between 2.51 and $2\sqrt{2}$, is not the diagonal of an upright quarter in the Q -system, then v does not affect the truncated cell $V_R(t_0)$ and may be disregarded. For this reason we confine our attention to upright diagonals, which by definition lie along an upright quarter in the Q -system.

3.2. Truncation.

We say that an upright diagonal $(0, v)$ can be *erased with penalty* $\pi_0 \geq 0$, if we have, in terms of the fine decomposition,

$$\sum_Q \sigma(Q) + \sum_S \sigma(V_S(t_S)) - 4\delta_{oct} \text{vol}(\delta_P(v)) < \pi_0 + \sum_Q \text{vor}_0(Q) + \sum_S \text{vor}_0(S).$$

Here the sum over Q runs over the upright quarters around $(0, v)$. Their scores $\sigma(Q)$ are context-dependent (see F.3.) The simplices S are those along $(0, v)$ of type S_C in the fine decomposition. We define their score $\sigma(V_S(t_S))$ as in Section 2. Also, $\delta_P(v)$ is the piece of the fine decomposition defined in Section 2. The right-hand side is scored by the truncation of the Voronoi function, Formula F.3.7. When we erase without mention of a penalty, $\pi_0 = 0$ is assumed.

If the diagonal can be erased, an upper bound on the score is obtained by ignoring the upright diagonal and all of the structures around it coming from the fine decomposition, and switching to the truncation at t_0 . Section 3 shows that various vertices can be erased, and this will greatly reduce the number combinatorial possibilities for an exceptional cluster.

3.3. Contexts.

Each upright diagonal has a context (p, q) , with p the number of anchors and $p - q$ the number of quarters around the diagonal [F]. The dihedral angle of a quarter is less than π (\mathbf{A}_8), so the context $(2, 0)$ is impossible. There is at least one quarter, so $p \geq q + 1$, $p \geq 2$.

The context $(2, 1)$ is treated in [F]. Proposition F.4.7 shows that by removing the upright diagonal, and scoring the surrounding region by a truncated version of the Voronoi function, an upper bound on the score is obtained. In the remaining contexts, $p \geq 3$. We start with contexts satisfying $p = 3$. The context $(3, 0)$ is to be regarded as two quasi-regular tetrahedra sharing a face rather than as three quarters along a diagonal. In particular, by [F], the upright quarters do not belong to the Q -system.

We recall that the score of an upright quarter is given by

$$\sigma(Q) = \nu(Q) = (\mu(Q) + \mu(\hat{Q}) + \text{vor}_0(Q) - \text{vor}_0(\hat{Q}))/2,$$

except in the contexts $(2, 1)$ and $(4, 0)$. The context $(2, 1)$ has been treated, and the context $(4, 0)$ does not occur in exceptional clusters. Thus, for the remainder of this paper, the scoring rule $\sigma(Q) = \nu(Q)$ will be used.

We have several different variants on the score depending on the truncation, analytic continuation, and so forth. If f is any of the functions

$$\text{vor}_0, \text{vor}, \Gamma, \nu,$$

we set $\tau_0, \tau_V, \tau_\Gamma, \tau_\nu$, respectively, to

$$\tau_* = -f(S) + \text{sol}(S)\zeta pt.$$

We set $\tau(S, t) = -\text{vor}(S, t) + \text{sol}(S)\zeta pt$. The family of functions τ_* measure what is squandered by a simplex. We say that Q has *compression type* or *Voronoi type* according to the scoring of $\mu(Q)$.

Crowns and anchor correction terms are used in [F] to erase upright quarters. We imitate those methods here. The functions *crown* and *anc* are defined and discussed in Section F.4. If $S = S(y_1, \dots, y_6)$ is a simplex along $(0, v)$, set

$$\kappa(S(y_1, \dots, y_6)) = \text{crown}(y_1/2) \text{dih}(S)/(2\pi) + \text{anc}(y_1, y_2, y_6) + \text{anc}(y_1, y_3, y_5).$$

$\kappa(S)$ is a bound on the difference in the score resulting from truncation around v . Assume that S is the simplex formed by $(0, v)$ and two consecutive anchors around $(0, v)$. Assume further that the circumradius of S is at least $\eta_0(y_1/2)$. Then we have

$$\kappa(S) = -4\delta_{\text{oct}} \text{vol}(\delta_P(W^e)),$$

where W^e is the extended wedge constructed in Section 2.3. To see this, it is a matter of interpreting the terms in κ . The function *crown* enters the volume through the region over the spherical cap D_0 of Section 2.3, lying outside $B(t_0)$. By multiplying by $\text{dih}(S)/(2\pi)$, we select the part of the spherical cap over the unextended wedge W between the anchors. The terms *anc* adjust for the four Rogers simplices lying above the extension W^e .

3.4. Three anchors.

Lemma 3.4.1. *The upright diagonal can be erased in the context $(3, 2)$.*

Proof. Let v_1 and v_2 be the two anchors of the upright diagonal $(0, v)$ along the quarter. Let the third anchor be v_3 .

Assume first that $|v| \geq 2.696$. If Q is of compression type, then by \mathbf{A}_{10} , the score is dominated by the truncated Voronoi function vor_0 . Assume Q is of Voronoi type. If $|v_1|, |v_2| \leq 2.45$, then \mathbf{A}_{11} gives the result. Take $|v_2| \geq 2.45$. By symmetry, $|v-v_1|$ or $|v-v_2| \geq 2.45$. The case $|v-v_1| \geq 2.45$ is treated by \mathbf{A}_{11} . We take $|v-v_2| \geq 2.45$. Let $S = (0, v, v_2, v_3)$. If S is of type S_C , the result follows from \mathbf{A}_{11} . (S is of type S_C , iff $y_4 \leq 2.77$, (because $\eta_{456} \geq \eta(2.45, 2, 2.77) > \sqrt{2}$.) If S is not of type S_C , we argue as follows. The function $h^2(\eta(2h, 2.45, 2.45)^{-2} - \eta_0(h)^{-2})$ is a quadratic polynomial in h^2 with negative values for $2h \in [2.696, 2\sqrt{2}]$. From this we find

$$\text{rad}(S) \geq \eta(2h, 2.45, 2.45) \geq \eta_0(h), \quad \text{where } 2h = |v|,$$

and this justifies the use of κ (see Section 2.3(2)). That the truncated Voronoi function dominates the score now follows from \mathbf{A}_9 .

Now assume that $|v| \leq 2.696$. If the simplices $(0, v, v_1, v_3)$ and $(0, v, v_2, v_3)$ are of type S_C , the bound follows from $\mathbf{A}_{10}, \mathbf{A}_{11}$. If say $S = (0, v, v_2, v_3)$ is not of type S_C , then

$$\text{rad}(S) \geq \sqrt{2} > \eta_0(2.696/2) \geq \eta_0(h),$$

justifying the use of κ . The bound follows from $\mathbf{A}_9, \mathbf{A}_{10}, \mathbf{A}_{11}$. ($\Gamma + \kappa < \text{octavor}_0$, etc.) \square

Lemma 3.4.2. *The upright diagonal can be erased in the context (3, 1), provided the three anchors do not form a flat quarter at the origin.*

Proof. In the absence of a flat quarter, truncate, score, and remove the vertex v as in the context (3, 1) of Proposition F.4.7. If there is a flat quarter, by the rules of [F], v is enclosed over the flat quarter. We do nothing further with them. This unerased case appears in the summary at the end of the section (3.10). \square

3.5. Six anchors.

Lemma. *An upright diagonal has at most five anchors.*

Proof. The proof relies on constants and inequalities from \mathbf{A}_3 and \mathbf{A}_8 . If between two anchors there is a quarter, then the angle is greater than 0.956, but if there is not, the angle is greater than 1.23. So if there are k quarters and at least six anchors, they squander more than

$$k(1.01104) - [2\pi - (6 - k)1.23]0.78701 > (4\pi\zeta - 8)pt,$$

for $k \geq 0$. \square

3.6. Anchored simplices.

Let $(0, v)$ be an upright diagonal, and let $v_1, v_2, \dots, v_k = v_1$ be its anchors, ordered cyclically around $(0, v)$. This cyclic order gives dihedral angles between consecutive anchors around the upright diagonal. We define the dihedral angles so that their sum is 2π , even though this will lead us to depart from our usual conventions by assigning a dihedral angle greater than π when all the anchors are concentrated in some half-space bounded by a plane through $(0, v)$. When the dihedral angle of $S = (0, v, v_i, v_{i+1})$ is at most π , we say that S is an *anchored simplex* if $|v_i - v_{i+1}| \leq 3.2$. (The constant 3.2 appears throughout this paper.) All upright quarters are anchored simplices. If an upright diagonal is completely surrounded by anchored simplices, the configuration of anchored simplices is sometimes called a *loop*. If $|v_i - v_{i+1}| > 3.2$ and the angle is less than π , we say there is a *large gap* around $(0, v)$ between v_i and v_{i+1} .

To understand how anchored simplices overlap we need a bound satisfied by vertices enclosed over an anchored simplex.

Lemma. *A vertex w of height between 2 and $2\sqrt{2}$, enclosed in the cone over an anchored simplex $(0, v, v_1, v_2)$ with diagonal $(0, v)$, satisfies $|w - v| \leq 2.51$. In particular, if $|w| \leq 2.51$, then w is an anchor.*

Proof. As in Lemma I.3.5, the vertex w cannot lie inside the anchored simplex. If $|v_1 - v_2| \leq 2\sqrt{2}$, the result follows from Lemma F.2.2 (or Lemma F.1.9). In

fact, if $|w| \leq 2\sqrt{2}$, the Voronoi cells at 0 and w meet, so that Lemma F.2.2 forces $(0, v_1, v_2, w)$ to be a quarter. (This observation gives a second proof of F.1.9.)

Assume that a figure exists with $|v_1 - v_2| > 2\sqrt{2}$. Suppose for a contradiction that $|v - w| > 2.51$. Pivot v_1 around $(0, v_2)$ until $|v - v_1| = 2.51$ and v_2 around $(0, v_1)$ until $|v - v_2| = 2.51$. Rescale w so that $|w| = 2\sqrt{2}$. Set $x = |v_1 - v_2|$. If, through geometric considerations, w is not deformed into the plane of $(0, v_2, v_1)$, then we are left with the one-dimensional family $|w'| = |w' - w| = 2$, for $w' = v_2, v_1$, $|v - w| = |v| = |v_1 - v| = |v_2 - v| = 2.51$, depending on x . This gives a contradiction

$$\begin{aligned} \pi &\geq \text{dih}(v_2, v_1, 0, v) + \text{dih}(v_2, v_1, v, w) \\ &= 2 \text{dih}(S(x, 2, 2.51, 2.51, 2.51, 2)) > \pi, \end{aligned}$$

for $x > 2\sqrt{2}$. (Equality is attained if $x = 2\sqrt{2}$.)

Thus, we may assume that w lies in the plane $P = (0, v_1, v_2)$. Take the circle in P at distance 2.51 from v . The vertices 0 and w lie on or outside the circle. The vertices v_1 and v_2 lie on the circle, so the diameter is at least $x > 2\sqrt{2}$. The distance from v to P is less than $x_0 = \sqrt{2.51^2 - 2}$. The edge $(0, w)$ cannot pass through the center of the circle, because $|w|$ is less than the diameter. Reflect v through P to get v' . Then $|v - v'| < 2x_0$. Swapping v_1 and v_2 as necessary, we may assume that w is enclosed over $(0, v, v', v_2)$. The desired bound $|v - w| \leq 2.51$ now follows from geometric considerations and the contradiction

$$2\sqrt{2} = |w| > \mathcal{E}(S(2, 2.51, 2.51, 2x_0, 2.51, 2.51), 2, 2.51, 2.51) = 2\sqrt{2}.$$

□

Corollary. *A vertex of height at most 2.51 is never enclosed over an anchored simplex.*

Proof. If so, it would be an anchor to the upright diagonal, contrary to the assumption that the anchored simplex is formed by consecutive anchors. □

3.7 Surrounded upright diagonals.

This proposition is a consequence of the two lemmas that follow. The context of the proposition is the set of anchored simplices that have not been erased by previous reductions.

Proposition. *Anchored simplices do not overlap.*

The remaining contexts have four or five anchors. Let w and the anchored simplex $S = (0, v, v_1, v_2)$ be as in Section 3.6. Our object is to describe the local geometry when an upright diagonal is enclosed over an anchored simplex. If $|v_1 - v_2| \leq 2\sqrt{2}$, we have seen in Section F.1.8 that there can be no enclosed upright diagonal with ≥ 4 anchors over the anchored simplex S .

Assume $|v_1 - v_2| > 2\sqrt{2}$. Let w_1, \dots, w_k , $k \geq 4$, be the anchors of $(0, w)$, indexed consecutively. The anchors of $(0, w)$ do not lie in $C(S)$, and the triangles $(0, w, w_i)$ and $(0, v, v_j)$ do not overlap. Thus, the plane $(0, v_1, v_2)$ separates w from $\{w_1, \dots, w_k\}$. Set $S_i = (0, w, w_i, w_{i+1})$. By **A**₈,

$$\pi \geq \text{dih}(S_1) + \dots + \text{dih}(S_{k-1}) \geq (k-1)0.956.$$

Thus, $k = 4$. The configuration of three simplices $\{S_i\}$, which we denote by \mathbf{S}_3^- , will be studied in the next two lemmas. The superscript reminds us that $\sum \text{dih}(S_i) - \pi$ is negative.

We claim that $\{v_1, v_2\} = \{w_1, w_4\}$. Suppose to the contrary that, after reindexing as necessary, $S_0 = (0, w, w_1, v_1)$ is a simplex, with $v_1 \neq w_1$, that does not overlap S_1, \dots, S_3 . Then $\pi \geq \text{dih}(S_0) + \dots + \text{dih}(S_3)$. So $0.28 \geq \pi - 3(0.956) \geq \text{dih}(S_0)$. \mathbf{A}_8 now implies that $|w - v_1| \geq 2\sqrt{2}$.

Assume that $(0, w, v_1, v_2)$ are coplanar. Disregard the other vertices. We minimize $|v_1 - v_2|$ when

$$|w| = 2\sqrt{2}, \quad |v_2| = |v_1| = |w - v_2| = 2, \quad |w - v_1| = 2\sqrt{2}.$$

This implies $3.2 \geq |v_1 - v_2| \geq x$, where x is the largest positive root of the polynomial $\Delta(8, 4, 4, x^2, 4, 8)$. But $x \approx 3.36$, a contradiction.

Since $(0, w, v_1, v_2)$ cannot be coplanar vertices, geometric considerations apply and

$$2\sqrt{2} \geq |w| \geq \mathcal{E}(S(2, 2, 2, 2, 2, 3.2), 2\sqrt{2}, 2, 2) > 2\sqrt{2}.$$

This contradiction establishes that $v_1 = w_1$.

Lemma 3.7.1. *If there is an upright diagonal $(0, v)$ with four anchors all concentrated in a half-space through $(0, v)$, then the three anchored simplices squander more than 0.5606 and score at most -0.4339 .*

Proof. The proof makes use of constants and inequalities from \mathbf{A}_2 , \mathbf{A}_8 , and \mathbf{A}_{12} . The dihedral angles are at most $\pi - 2(0.956) < 1.23$. This forces $y_4 \leq 2.51$, for each simplex S . So they are all quarters. The three anchored simplices squander at least

$$3(1.01104) - \pi(0.78701) > 0.5606.$$

The bound on score follows similarly from $\nu < -0.9871 + 0.80449 \text{ dih}$. \square

Lemma 3.7.2. *If an \mathbf{S}_3^- configuration overlaps an anchored simplex, the decomposition star squanders at least $(4\pi\zeta - 8)$ pt.*

Proof. Suppose that $(0, v, v_1, v_2)$ is an anchored simplex that another anchored simplex overlaps, with $(0, v)$ the upright diagonal. Let $(0, w)$ be the upright diagonal of an \mathbf{S}_3^- configuration. We score the two simplices $S'_i = (0, v, w, v_i)$ by truncation at $\sqrt{2}$. Truncation at $\sqrt{2}$ is justified by face-orientation arguments or by geometric considerations:

$$\mathcal{E}(S(2, 2.51, 2.51, 2.51, 2.51, 2.51), 2, 2, 2) > 2\sqrt{2}.$$

By \mathbf{A}_{12} ,

$$\tau_V(S'_1, \sqrt{2}) + \tau_V(S'_2, \sqrt{2}) \geq 2(0.13) + 0.2(\text{dih}(S'_1) + \text{dih}(S'_2) - \pi) > 0.26.$$

Together with the three simplices in \mathbf{S}_3^- that squander at least 0.5606, we obtain the stated bound. \square

3.8. Five anchors.

When there are five anchors of an upright diagonal, each dihedral angle around the diagonal is at most $2\pi - 4(0.956) < \pi$. There are at most two large gaps by \mathbf{A}_8 ,

$$3(1.65) + 2(0.956) > 2\pi.$$

Lemma 3.8.1. *If an upright diagonal has five anchors with two large gaps, then the three anchored simplices squander $> (4\pi\zeta - 8)$ pt.*

Proof. By \mathbf{A}_8 , the anchored simplices are all quarters, $1.23 + 2(1.65) + 2(0.956) > 2\pi$. The dihedral angle is less than $2\pi - 2(1.65)$. The linear programming bound from \mathbf{A}_3 is greater than $0.859 > (4\pi\zeta - 8)$ pt. \square

Define a *masked* flat quarter to be a flat quarter that is not in the Q -system because it overlaps an upright quarter in the Q -system. They can only occur in a very special setting.

Lemma 3.8.2. *Let $(0, v)$ be an upright diagonal with at least four anchors. If Q is a flat quarter that overlaps an anchored simplex that lies along $(0, v)$, then the vertices of Q are the origin and three consecutive anchors of $(0, v)$.*

Proof. For there to be overlap, the diagonal (w_1, w_2) of Q must pass through the face $(0, v, v_1)$ formed by some anchor v_1 . (see Lemma F.1.3). By Lemma F.1.5, w_1 and w_2 are anchors of $(0, v)$. By Lemma F.1.8, w_2, v_1 , and w_1 are consecutive anchors. If v_1 is a vertex of Q we are done. Otherwise, let $w_3 \neq 0, w_1, w_2$ be the remaining vertex of Q . The edges (v, v_1) and $(v_1, 0)$ do not pass through the face (w_1, w_2, w_3) by Lemma F.1.3. Likewise, the edges (w_2, w_3) and (w_3, w_1) do not pass through the face $(0, v, v_1)$. Thus, v is enclosed over the quarter Q .

Let $w'_3 \neq w_1, v_1, w_2$ be a fourth anchor of $(0, v)$. By Lemma F.1.3, we have $w'_3 = w_3$. \square

Corollary (of proof). *If v is enclosed over a flat quarter, then $(0, v)$ has at most four anchors.* \square

When we are unable to erase the upright diagonal with five anchors and a large gap, we are able to obtain strong bounds on the score. We let \mathbf{S}_4^+ denote the configuration of four upright quarters and the large gap around an upright diagonal.

Lemma 3.8.3. *Suppose an upright diagonal has five anchors and one large gap. The four anchored simplices score at most -0.25 . The four anchored simplices squander at least 0.4 . If any of the four anchored simplices is not an upright quarter then the four simplices squander at least $(4\pi\zeta - 8)$ pt.*

Proof. \mathbf{A}_2 and $\text{dih} > 1.65$ from \mathbf{A}_8 give the bound -0.25 . \mathbf{A}_3 gives the bound 0.4 . To get the final statement of the lemma, use inequalities \mathbf{A}_5 and \mathbf{A}_7 as well. \square

Corollary. *There is at most one \mathbf{S}_4^+ .*

Proof. The crown along the large gap, with the bound of the lemma, gives $0.4 - \kappa \geq 0.4 + 0.02274$ squandered by each \mathbf{S}_4^+ (see \mathbf{A}_9). The rest squanders a positive amount (see Lemma 4.1). If there are two \mathbf{S}_4^+ -configurations, use $2(0.4 + 0.02274) > (4\pi\zeta - 8)$ pt. \square

We set $\xi_\Gamma = 0.01561$, $\xi_V = 0.003521$, $\xi'_\Gamma = 0.00935$, $\xi_\kappa = -0.029$, $\xi_{\kappa, \Gamma} = \xi_\kappa + \xi_\Gamma = -0.01339$. The first two constants appear in \mathbf{A}_{10} and \mathbf{A}_{11} as penalties for erasing upright quarters of compression type, and Voronoi type, respectively. ξ'_Γ is an improved bound on the penalty for erasing when the upright diagonal is at least 2.57 . Also, ξ_κ is an upper bound on κ from \mathbf{A}_9 , when the upright diagonal is at most 2.57 . If the upright diagonal is at least 2.57 , then we still obtain the bound $\xi_{\kappa, \Gamma} = -0.02274 + \xi'_\Gamma$ from \mathbf{A}_9 on the sum of κ with the penalty from erasing an upright quarter.

3.9. Four anchors.

Lemma 3.9.1. *If there are at least two large gaps around an upright diagonal with 4 anchors, then it can be erased.*

Proof. There are at least as many large gaps as upright quarters. Each large gap drops us by ξ_κ and each quarter lifts us by at most ξ_Γ by $\mathbf{A}_9, \mathbf{A}_{10}, \mathbf{A}_{11}$. We have $\xi_{\kappa, \Gamma} < 0$. \square

Remark. *Let $(0, v)$ be an enclosed vertex over a flat quarter. Then*

$$|v| \geq \mathcal{E}(2, 2, 2, 2.51, 2.51, 2\sqrt{2}, 2, 2, 2) > 2.6.$$

If an edge of the flat quarter is sufficiently short, say $y_6 \leq 2.2$, then

$$|v| \geq \mathcal{E}(2, 2, 2, 2.2, 2.51, 2\sqrt{2}, 2, 2, 2) > 2.7.$$

The two dihedral angles on the gaps are > 1.65 . If the two quarters mask a flat quarter, we use the scoring of 3.10.2.c. We have $0.0114 < -2\xi_{\kappa, \Gamma}$.

When there is one large gap, we may erase with a penalty $\pi_0 = 0.008$.

Lemma 3.9.2. *Let v be an upright diagonal with 4 anchors. Assume that there is one large gap. The anchored simplices can be erased with penalty $\pi_0 = 0.008$. If any of the anchored simplices around v is not an upright quarter then we can erase with penalty $\pi_0 = 0.00222$.*

Moreover, if there is a flat quarter overlapping an upright quarter, then (1) or (2) holds.

(1) The truncated Voronoi function exceeds the score by at least 0.0063. The diagonal of the flat is at least 2.6, and the edge opposite the diagonal is at least 2.2.

(2) The truncated Voronoi function exceeds the score by at least 0.0114. The diagonal of the flat is at least 2.7, and the edge opposite the diagonal is at most 2.2.

As a matter of notation, we let \mathbf{S}_3^+ be the configuration of three simplices described by the lemma, when there is no masked flat quarter.

Proof. The constants and inequalities used in this proof can be found in $\mathbf{A}_9, \mathbf{A}_{10}$, and \mathbf{A}_{11} .

First we establish the penalty 0.008. The truncated Voronoi function is an upper bound on the score of an anchored simplex that is not a quarter. By these inequalities, the result follows if the diagonal satisfies $y_1 \geq 2.57$. Take $y_1 \leq 2.57$.

If any of the upright quarters are of Voronoi type, the result follows from $(\xi_{\kappa, \Gamma} + \xi_\Gamma < 0.008)$. If the edges along the large gap are less than 2.25, the result follows from $(-0.03883 + 3\xi_\Gamma = 0.008)$. If all but one edge along the large gap are less than 2.25, the result follows from $(-0.0325 + 2\xi_\Gamma + 0.00928 = 0.008)$.

If there are at least two edges along the large gap of length at least 2.25, we consider two cases according to whether they lie on a common face of an upright quarter. The same group of inequalities from the appendix gives the result. The bound 0.008 is now fully established.

Next we prove that we can erase with penalty 0.00222, when one of the anchored simplices is not a quarter. If $|v| \geq 2.57$, then we use

$$2\xi_\Gamma + \xi_V + \xi_\kappa \leq 0.00935 + 0.003521 - 0.2274 \leq 0.$$

If $|v| \leq 2.57$, we use

$$2(0.01561) - 0.029 \leq 0.00222.$$

Let $v_1 \dots, v_4$ be the consecutive anchors of the upright diagonal $(0, v)$ with (v_1, v_4) the large gap. Suppose $|v_1 - v_3| \leq 2\sqrt{2}$.

We claim the upright diagonal $(0, v)$ is not enclosed over $(0, v_1, v_2, v_3)$. Assume the contrary. The edge (v_1, v_3) passes through the face $(0, v, v_4)$. Disregarding the vertex v_2 , by geometric considerations, we arrive at the rigid figure

$$\begin{aligned} |v| &= 2\sqrt{2}, \quad |v_1| = |v_1 - v| = |v - v_3| = |v_3| = |v_3 - v_4| = 2 \\ |v - v_4| &= |v_4| = 2.51, \quad |v_1 - v_4| = 3.2. \end{aligned}$$

The dihedral angles of $(0, v, v_1, v_4)$ and $(0, v, v_3, v_4)$ are

$$\text{dih}(S(2\sqrt{2}, 2, 2.51, 3.2, 2.51, 2)) > 2.3, \quad \text{dih}(S(2\sqrt{2}, 2, 2.51, 2, 2.51, 2)) > 1.16$$

The sum is greater than π , contrary to the claim that the edge (v_1, v_3) passes through the face $(0, v, v_4)$. (This particular conclusion leads to the corollary cited at the end of the proof.) Thus, (v_1, v_3) passes through $(0, v, v_2)$ so that the simplices $(0, v, v_1, v_2)$ and $(0, v, v_2, v_3)$ are of Voronoi type.

To complete the proof of the lemma, we show that when there is a masked flat quarter, either (1) or (2) holds. Suppose we mask a flat quarter $Q' = (0, v_1, v_2, v_3)$. We have established that (v_1, v_3) passes through the face $(0, v, v_2)$. To establish (1) assume that $|v_2| \geq 2.2$. The remark before the lemma gives

$$|v_1 - v_3| \geq \mathcal{E}(S(2, 2, 2, 2\sqrt{2}, 2.51, 2.51), 2, 2, 2) > 2.6.$$

The bound 0.0063 comes from

$$\xi_{\kappa, \Gamma} + 2\xi_V < -0.0063$$

To establish (2) assume that $|v_2| \leq 2.2$. The remark gives

$$|v_1 - v_3| \geq \mathcal{E}(S(2, 2, 2, 2\sqrt{2}, 2.2, 2.51), 2, 2, 2) > 2.7.$$

If the simplex $(0, v, v_3, v_4)$ is of Voronoi type, then

$$\xi_{\kappa} + 3\xi_V < -0.0114$$

Assume that $(0, v, v_3, v_4)$ is of compression type. We have

$$-0.004131 + \xi_{\kappa, \Gamma} + \xi_V \leq -0.0114.$$

□

Corollary (of proof). *If there are four anchors and if the upright diagonal is enclosed over a flat quarter, then there are four anchored simplices and at least three quarters around the upright diagonal.* □

3.10. Summary.

The following index summarizes the cases of upright quarters that have been treated in Section 3. If the number of anchors is the number of anchored simplices (no large gaps), the results appear in Section 5.11. Every other possibility has been treated.

- 0,1,2 anchors Sec. 3.3
- 3 anchors Sec. 3.4
 - context (3, 0)
 - context (3, 1)
 - context (3, 2)
 - context (3, 3)
- 4 anchors Sec. 3.9
 - 0 gaps (Section 5.11)
 - 1 gap
 - 2 or more gaps
- 5 anchors Sec. 3.8
 - 0 gaps (Section 5.11)
 - 1 gap (\mathbf{S}_4^+)
 - 2 or more gaps
- 6 or more anchors Sec. 3.5

By truncation and various comparison lemmas, we have entirely eliminated upright diagonals except when there are between three and five anchors. We may assume that there is at most one large gap around the upright diagonal.

1. Consider an anchored simplex Q around a remaining upright diagonal. The score of is $\nu(Q)$ if Q is a quarter, the analytic Voronoi function $\text{vor}(Q)$ if the simplex is of type S_C (Section 2.5), and the truncated Voronoi function $\text{vor}_0(Q)$ otherwise.

2. Consider a flat quarter Q in an exceptional cluster. An upper bound on the score is obtained by taking the maximum of all of the following functions that satisfy the stated conditions on Q . Let y_4 denote the length of the diagonal and y_1 be the length of the opposite edge.

- (a) The function $\mu(Q)$.
- (b) $\text{vor}_0(Q) - 0.0063$, if $y_4 \geq 2.6$ and $y_1 \geq 2.2$. (Lemma 3.9)
- (c) $\text{vor}_0(Q) - 0.0114$, if $y_4 \geq 2.7$ and $y_1 \leq 2.2$. (Lemma 3.9)
- (d) $\nu(Q_1) + \nu(Q_2) + \text{vor}_x(S)$, if there is an enclosed vertex v over Q of height between 2.51 and $2\sqrt{2}$ that partitions the convex hull of (Q, v) into two upright quarters Q_1 , Q_2 and a third simplex S . Here $\text{vor}_x = \text{vor}$ if S is of type S_C , and $\text{vor}_x = \text{vor}_0$ otherwise. (Lemma 3.4)
- (e) $\text{vor}(Q, 1.385)$ if the simplex is of type S_B (Section 2.5).
- (f) $\text{vor}_0(Q)$ if the simplex is an isolated quarter with $\max(y_2, y_3) \geq 2.23$, $y_4 \geq 2.77$, and $\eta_{456} \geq \sqrt{2}$.

3. If S is a simplex is of type S_A , its score is $\text{vor}(S)$. (Section 2.5.)

4. Everything else is scored by the truncation of Voronoi, vor_0 . The Formula F.3.7 is used on these remaining pieces. On top of what is obtained for the standard cluster by summing all these terms, there is a penalty $\pi_0 = 0.008$ each time the simplex configuration \mathbf{S}_3^+ is erased.

5. The remaining upright diagonals not surrounded by anchored simplices are \mathbf{S}_3^+ , \mathbf{S}_3^- , \mathbf{S}_4^+ from Section 3.7, 3.8 and 3.9.

3.11. Some flat quarters.

Recall that $\xi_V = 0.003521$, $\xi_\Gamma = 0.01561$, $\xi'_\Gamma = 0.00935$. They are the penalties that result from erasing an upright quarter of Voronoi type, an upright quarter of compression type, and an upright quarter of compression type with diagonal ≥ 2.57 . (See \mathbf{A}_{10} and \mathbf{A}_{11} .)

In the next lemma, we score a flat quarter by any of the functions on the given domains

$$\hat{\sigma} = \begin{cases} \Gamma, & \eta_{234}, \eta_{456} \leq \sqrt{2}, \\ \text{vor}, & \eta_{234} \geq \sqrt{2}, \\ \text{vor}_0, & y_4 \geq 2.6, y_1 \geq 2.2, \\ \text{vor}_0, & y_4 \geq 2.7, \\ \text{vor}_0, & \eta_{456} \geq \sqrt{2}. \end{cases}$$

Lemma 3.11.1. *$\hat{\sigma}$ is an upper bound on the functions in Section 3.10(a)–(f). That is, each function in Section 3.10 is dominated by some choice of $\hat{\sigma}$.*

Proof. The only case in doubt is the function of 3.10(d):

$$\nu(Q_1) + \nu(Q_2) + \text{vor}_x(S).$$

This is established by the following lemma. \square

We consider the context (3, 1) that occurs when two upright quarters in the Q -system lie over a flat quarter. Let $(0, v)$ be the upright diagonal, and assume that $(0, v_1, v_2, v_3)$ is the flat quarter, with diagonal (v_2, v_3) . Let σ denote the score of the upright quarters and other anchored simplex lying over the flat quarter.

Lemma 3.11.2. $\sigma \leq \min(0, \text{vor}_0)$.

Proof. The bound of 0 is established in [II] and [F].

By F.4.7.5, if $|v| \geq 2.69$, then the upright quarters satisfy

$$\nu < \text{vor}_0 + 0.01(\pi/2 - \text{dih})$$

so the upright quarters can be erased. Thus we assume without loss of generality that $|v| \leq 2.69$.

We have

$$|v| \geq \mathcal{E}(S(2, 2, 2, 2t_0, 2t_0, 2\sqrt{2}), 2, 2, 2) > 2.6.$$

If $|v_1 - v_2| \leq 2.1$, or $|v_1 - v_3| \leq 2.1$, then

$$|v| \geq \mathcal{E}(S(2, 2, 2, 2.1, 2t_0, 2\sqrt{2}), 2, 2, 2) > 2.72,$$

contrary to assumption. So take $|v_1 - v_2| \geq 2.1$ and $|v_1 - v_3| \geq 2.1$. Under these conditions we have the interval calculation $\nu(Q) < \text{vor}_0(Q)$ where Q is the upright quarter (see \mathbf{A}_{13}). \square

Remark. *If we have an upright diagonal enclosed over a masked flat quarter in the context (4, 1), then there are 3 upright quarters. By the same argument as in the lemma, the two quarters over the masked flat quarter score $\leq \text{vor}_0$. The third quarter can be erased with penalty ξ_V .*

Define the *central vertex* v of a flat quarter to be the vertex for which $(0, v)$ is the edge opposite the diagonal.

Lemma 3.11.3. $\mu < \text{vor}_0 + 0.0268$ for all flat quarters. If the central vertex has height ≤ 2.17 , then $\mu < \text{vor}_0 + 0.02$.

Proof. This is an interval calculation. See **A**₁₃. \square

We measure what is squandered by a flat quarter by $\hat{\tau} = \text{sol } \zeta pt - \hat{\sigma}$.

Lemma 3.11.4. Let v be a corner of an exceptional cluster at which the dihedral angle is at most 1.32. Then the vertex v is the central vertex of a flat quarter Q in the exceptional region. Moreover, $\hat{\tau}(Q) > 3.07 \text{ pt}$. If $\hat{\sigma} = \text{vor}_0$ (and if $\eta_{456} \geq \sqrt{2}$), we may use the stronger constant $\tau_0(Q) > 3.07 \text{ pt} + \xi_V + 2\xi'_F$.

Proof. Let $S = S(y_1, \dots, y_6)$ be the simplex inside the exceptional cluster centered at v , with $y_1 = |v|$. The inequality $\text{dih} \leq 1.32$ gives the interval calculation $y_4 \leq 2\sqrt{2}$, so S is a quarter. The result now follows by interval arithmetic. See **A**₁₃. \square

4. DISTINGUISHED EDGES AND SUBREGIONS

4.1. Positivity.

Lemma. $\tau_0 \geq 0$ on local V -cells.

Proof. Everything truncated at t_0 can be broken into three types of pieces: Rogers simplices $R(a, b, t_0)$, wedges of t_0 -cones, and spherical regions. (See Diagram II.4.2.) The wedges of t_0 -cones and spherical regions can be considered as the degenerate cases $b = t_0$ and $a = b = t_0$ of Rogers simplices, so it is enough to show that $\tau(R(a, b, t_0)) \geq 0$. We have $t_0 > \sqrt{3/2}$, so by Rogers's lemma (I.8.6.2),

$$\tau(R(a, b, t_0)) > \tau(R(1, \eta(2, 2, 2), \sqrt{3/2})).$$

The right-hand side is zero. (In fact, the vanishing of the right-hand side is essentially Rogers's bound. Nothing is squandered when Rogers's bound is met.) \square

4.2. Distinguished edge conditions.

Take an exceptional cluster. We prepare the cluster by erasing all upright diagonals possible, including the \mathbf{S}_3^+ , \mathbf{S}_4^+ , \mathbf{S}_3^- configurations. The only remaining upright diagonals are those on an upright diagonal surrounded by anchored simplices (loops). When the upright diagonal is erased, we score with the truncated Voronoi function. The exceptional clusters in Sections 4 and 5 are assumed to be prepared in this way.

A simplex S is *special* if the fourth edge has length at least $2\sqrt{2}$ and at most 3.2, and the others have length at most 2.51. The fourth edge will be called its diagonal.

We draw a system of edges between vertices. Each vertex will have height at most 2.51. The projections of the edges to the unit sphere will divide the standard region into subregions. We call an edge *nonexternal* if the projection of the edge lies entirely in the (closed) exceptional region.

1. Draw all nonexternal edges of length at most $2\sqrt{2}$ except those between nonconsecutive anchors of a remaining upright diagonal. These edges do not cross (Lemma F.1.6). These edges do not cross the edges of anchored simplices (Lemmas 3.6, F.1.5).

2. Draw all edges of (remaining) anchored upright simplices that are opposite the upright diagonal, except when the edge gives a special simplex. The anchored simplices do not overlap (Lemma 3.7), so these edges do not cross. These edges are nonexternal (Lemma 3.6, F.1.3).

3. Draw as many additional nonexternal edges as possible of length at most 3.2 subject to not crossing another edge, not crossing any edge of an anchored simplex, and not being the diagonal of a special simplex.

We fix once and for all a maximal collection of edges subject to these constraints. Edges in this collection are called *distinguished* edges. The projection of the distinguished edges to the unit sphere gives the bounding edges of regions called the *subregions*. Each standard region is a union of subregions. The vertices of height at most 2.51 and the vertices of the remaining upright diagonals are said to form a *subcluster*.

By construction, the special simplices and anchored simplices around an upright quarter form a subcluster. Flat quarters in the Q -system, flat quarters of an isolated pair, and simplices of type S_A and S_B are subclusters. Other subclusters are scored

by the truncation of the Voronoi function. For these subclusters, the Formula F.3.7 extends without modification.

4.3. Scoring subclusters.

The terms of Equation F.3.7 defining $\text{vor}_0(P) = \text{vor}(P, t_0)$ have a clear geometric interpretation as quoins, wedges of t_0 -cones, and solid angles (see [F]). There is a quoin for each Rogers simplex. There is a somewhat delicate point that arises in connection with the geometry of subclusters. It is not true in general that the Rogers simplices entering into the truncation $\text{vor}_0(P)$ of P lie in the cone over P . Formula F.3.7 should be viewed as an analytic continuation that has a nice geometric interpretation when things are nice, and which always gives the right answer when summed over all the subclusters in the cluster, but which may exhibit unusual behavior in general. The following lemma shows that the simple geometric interpretation of Formula F.3.7 is valid when the subregion is not triangular.

Lemma. *If a subregion is not a triangle and is not the subregion containing the anchored simplices around an upright diagonal, the cone of arcradius*

$$\psi = \arccos(|v|/2.51)$$

centered along $(0, v)$, where v is a corner of the subcluster, does not cross out of the subregion.

Proof. For a contradiction, let (v_1, v_2) be a distinguished edge that the cone crosses. If both edges (v, v_1) and (v, v_2) have length less than 2.51, there can be no enclosed vertex w of height at most 2.51, unless its distance from v_1 and v_2 is less than 2.51:

$$\mathcal{E}(S(2, 2, 2, 2.51, 2.51, 3.2), 2.51, 2, 2) > 2.51.$$

In this case, we can replace (v_1, v_2) by an edge of the subregion closer to v , so without loss of generality we may assume that there are no enclosed vertices when both edges (v, v_1) and (v, v_2) have length less than 2.51.

The subregion is not a triangle, so $|v - v_1| \geq 2.51$, or $|v - v_2| \geq 2.51$, say $|v - v_1| \geq 2.51$. Also $|v - v_2| \geq 2$. Pivot so that $|v_1 - v_2| = 3.2$, $|v - v_1| = 2.51$, $|v - v_2| = 2$. (The simplex $(0, v_1, v_2, v)$ cannot collapse ($\Delta \neq 0$) as we pivot. See Inequality 4.8(*) below.) Then use $\beta_\psi \leq \text{dih}_3$ from **A**₁. \square

As a consequence, in nonspecial standard regions, the terms in the Formula F.3.7 for vor_0 retain their interpretations as quoins, Rogers simplices, t_0 -cones, and solid angles, all lying in the cone over the standard region.

4.4. The main theorem.

Let R be a standard cluster. Let U be the set of corners, that is, the set of vertices in the cone over R that have height at most 2.51. Consider the set E of edges of length at most 2.51 between vertices of U . We attach a multiplicity to each edge. We let the multiplicity be 2 when the edge projects to the interior of the standard region, and 0 when the edge projects to the complement of the standard region. The other edges, those bounding the standard region, are counted with multiplicity 1.

Let n_1 be the number of edges in E , counted with multiplicities. Let c be the number of classes of vertices under the equivalence relation $v \sim v'$ if there is a sequence of edges in E from v to v' . Let $n(R) = n_1 + 2(c - 1)$. If the standard region under R is a polygon, then $n(R)$ is the number of sides.

Theorem. $\tau(R) > t_n$, where $n = n(R)$ and

$$\begin{aligned} t_4 &= 0.1317, & t_5 &= 0.27113, & t_6 &= 0.41056, \\ t_7 &= 0.54999, & t_8 &= 0.6045. \end{aligned}$$

The decomposition star scores less than 8 *pt*, if $n(R) \geq 9$, for some standard cluster R . The scores satisfy $\sigma(R) < s_n$, for $5 \leq n \leq 8$, where

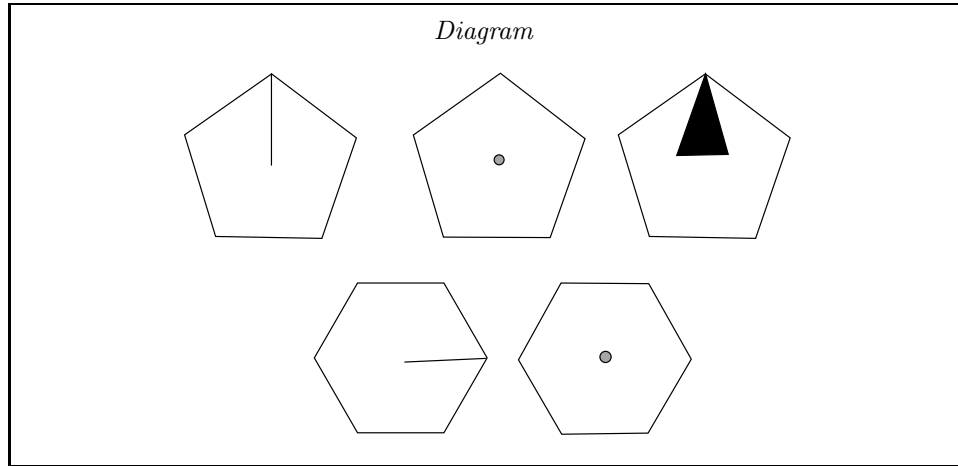
$$s_5 = -0.05704, \quad s_6 = -0.11408, \quad s_7 = -0.17112, \quad s_8 = -0.22816.$$

Sometimes, it is convenient to calculate these bounds as a multiple of *pt*. We have

$$\begin{aligned} t_4 &> 2.378 \text{ pt}, & t_5 &> 4.896 \text{ pt}, & t_6 &> 7.414 \text{ pt}, \\ t_7 &> 9.932 \text{ pt}, & t_8 &> 10.916 \text{ pt}. \end{aligned}$$

$$s_5 < -1.03 \text{ pt}, \quad s_6 < -2.06 \text{ pt}, \quad s_7 < -3.09 \text{ pt}, \quad s_8 < -4.12 \text{ pt}.$$

Corollary. Every standard region is either a polygon or one shown in the diagram.



In the cases that are not (simple) polygons, we call the *polygonal hull* the polygon obtained by removing the internal edges and vertices. We have $m(R) \leq n(R)$, where the constant $m(R)$ is the number of sides of the polygonal hull.

Proof. By the theorem, if the standard region is not a polygon, then $8 \geq n_1 \geq m \geq 5$. (Quad clusters and quasi-regular tetrahedra have no enclosed vertices. See Lemma I.3.7 and Lemma III.2.2.) If $c > 1$, then $8 \geq n = n_1 + 2(c-1) \geq 5 + 2(c-1)$, so $c = 2$, and $n_1 = 5, 6$ (frames 2 and 5 of the diagram).

Now take $c = 1$. Then $8 \geq n \geq 5 + (n - m)$, so $n - m \leq 3$. If $n - m = 3$, we get frame 3. If $n - m = 2$, we have $8 \geq m + 2 \geq 5 + 2$, so $m = 5, 6$ (frames 1, 4).

But $n - m = 1$ cannot occur, because a single edge that does not bound the polygonal hull has even multiplicity. Finally, if $n - m = 0$, we have a polygon. \square

4.5. Proof.

The proof of the theorem occupies the rest of the paper. We begin with a slightly simplified account of the method of proof. Set $t_9 = 0.6978$, $t_{10} = 0.7891$, $t_n = (4\pi\zeta - 8)pt$, for $n \geq 11$. Set $D(n, k) = t_{n+k} - 0.06585k$, for $0 \leq k \leq n$, and $n + k \geq 4$. This function satisfies

$$(4.5.1) \quad D(n_1, k_1) + D(n_2, k_2) \geq D(n_1 + n_2 - 2, k_1 + k_2 - 2).$$

In fact, this inequality unwinds to $t_r + 0.13943 \geq t_{r+1}$, $D(3, 2) = 0.13943$, and $t_n = (0.06585)2 + (n - 4)D(3, 2)$, for $n = 4, 5, 6, 7$. These hold by inspection.

Call an edge between two vertices of height at most 2.51 *long* if it has length greater than 2.51. Add the distinguished edges to break the standard regions into subregions. We say that a subregion has *edge parameters* (n, k) if there are n bounding edges, where k of them are long. (We count edges with multiplicities as in Section 4.4, if the subregion is not a polygon.) Combining two subregions of edge parameters (n_1, k_1) and (n_2, k_2) along a long edge e gives a union with edge parameters $(n_1 + n_2 - 2, k_1 + k_2 - 2)$, where we agree not to count the internal edge e that no longer bounds. Inequality 4.5.1 localizes the main theorem to what is squandered by subclusters. Suppose we break the standard cluster into groups of subregions such that if the group has edge parameters (n, k) , it squanders at least $D(n, k)$. Then by superadditivity (4.5.1), the full standard cluster R must squander $D(n, 0) = t_n$, $n = n(R)$, giving the result.

Similarly, define constants $s_4 = 0$, $s_9 = -0.1972$, $s_n = 0$, for $n \geq 10$. Set $Z(n, k) = s_{n+k} - k\epsilon$, for $(n, k) \neq (3, 1)$, and $Z(3, 1) = \epsilon$, where $\epsilon = 0.00005$ (cf. **A**₁). The function $Z(n, k)$ is subadditive:

$$Z(n_1, k_1) + Z(n_2, k_2) \leq Z(n_1 + n_2 - 2, k_1 + k_2 - 2).$$

In fact, this easily follows from $s_a + s_b \leq s_{a+b-4}$, for $a, b \geq 4$, and $\epsilon > 0$. It will be enough in the proof of Theorem 4.4 to show that the score of a union of subregions with edge parameters (n, k) is at most $Z(n, k)$.

4.6. Nonagons.

A few additional comments are needed to eliminate $n = 9, 10$, even after the bounds t_9, t_{10} are established. Suppose that $n = 9$, and that R squanders at least t_9 and scores less than s_9 . This bound is already sufficient to conclude that there are no other standard clusters except quasi-regular tetrahedra ($t_9 + t_4 > (4\pi\zeta - 8)pt$). There are no vertices of type $(4, 0)$ or $(6, 0)$: $t_9 + 4.14pt > (4\pi\zeta - 8)pt$ [III.5.2]. So all vertices not over the exceptional cluster are of type $(5, 0)$. Suppose that there are ℓ vertices of type $(5, 0)$. The polygonal hull of R has $m \leq 9$ edges. There are $m - 2 + 2\ell$ quasi-regular tetrahedra. If $\ell \leq 3$, then by III.5.3, the score is less than

$$s_9 + (m - 2 + 2\ell)pt - 0.48\ell pt < 8pt.$$

If on the other hand, $\ell \geq 4$, the decomposition star squanders more than

$$t_9 + 4(0.55)pt > (4\pi\zeta - 8)pt.$$

The bound s_9 will be established as part of the proof of Theorem 4.4.

The case $n = 10$ is similar. If $\ell = 0$, the score is less than $(m - 2)pt \leq 8pt$, because the score of an exceptional cluster is strictly negative, [F.3.13]. If $\ell > 0$, we squander at least $t_{10} + 0.55pt > (4\pi\zeta - 8)pt$ (III.5.3).

4.7 Preparation of the standard cluster.

Fix a standard cluster. We return to the construction of subregions and distinguished edges, to describe the penalties. Take the penalty of 0.008 for \mathbf{S}_3^+ . Take the penalty $0.03344 = 3\xi_\Gamma + \xi_{\kappa,\Gamma}$ for \mathbf{S}_4^+ . Take the penalty $0.04683 = 3\xi_\Gamma$ for \mathbf{S}_3^- . Set $\pi_{\max} = 0.06688$. The penalty in the next lemma refers to the combined penalty from erasing all \mathbf{S}_3^- , \mathbf{S}_3^+ , and \mathbf{S}_4^+ configurations in the decomposition star. The upright quarters that completely surround an upright diagonal (loops) are not erased.

Lemma. *The total penalty from a decomposition star is at most π_{\max} .*

Proof. Before any upright quarters are erased, each quarter squanders > 0.033 (\mathbf{A}_{13}), so the star squanders $> (4\pi\zeta - 8) pt$ if there are ≥ 25 quarters. Assume there are at most 24 quarters. If the only penalties are 0.008, we have $8(0.008) < \pi_{\max}$. If we have the penalty 0.04683, there are at most 7 other quarters ($0.5606 + 8(0.033) > (4\pi\zeta - 8) pt$) (Lemma 3.7), and no other penalties from this type or from \mathbf{S}_4^+ , so the total penalty is at most $2(0.008) + 0.04683 < \pi_{\max}$. Finally, if there is one context \mathbf{S}_4^+ , there are at most 12 other quarters (Section 3.8), and erasing gives the penalty $0.03344 + 4(0.008) < \pi_{\max}$. \square

The remaining upright diagonals are surrounded by anchored simplices. If the edge opposite the diagonal in an anchored simplex has length $\geq 2\sqrt{2}$, then there may be an adjacent special simplex whose diagonal is that edge. Section 5.11 will give bounds on the aggregate of these anchored simplices and special simplices. In all other contexts, the upright quarters have been erased with penalties.

Break the standard cluster into subclusters as in Section 4.2. If the subregion is a triangle, we refer to the bounds of 5.7. Sections 4.8–5.10 give bounds for subregions that are not triangles in which all the upright quarters have been erased. We follow the strategy outlined in Section 4.5, although the penalties will add certain complications.

We now assume that we have a subcluster without quarters and whose region is not triangular. The truncated Voronoi function vor_0 is the score. Penalties are largely disregarded until Section 5.4.

We describe a series of deformations of the subcluster that increase vor_0 and decrease τ_0 . These deformations disregard the broader geometric context of the subcluster. Consequently, we cannot claim that the deformed subcluster exists in any decomposition star. As the deformation progresses, an edge (v_1, v_2) , not previously distinguished, can emerge with the properties of a distinguished edge. If so, we add it to the collection of distinguished edges, use it if possible to divide the subcluster into smaller subclusters, and continue to deform the smaller pieces. When triangular regions are obtained, they are set aside until Section 5.7.

4.8 Reduction to polygons.

By deformation, we can produce subregions whose boundary is a polygon. Let U be the set of vertices over the subregion of height ≤ 2.51 . As in Section 4.4, the distinguished edges partition U into equivalence classes. Move the vertices in one equivalence class U_1 as a rigid body preserving heights until the class comes sufficiently close to form a distinguished edge with another subset. Continue until all the vertices are interconnected by paths of distinguished edges. vor_0 and τ_0 are unchanged by these deformations.

If some vertex v is connected to three or more vertices by distinguished edges, it follows from the connectedness of the open subregion that there is more than one connected component U_i (by paths of distinguished edges) of $U \setminus \{v\}$. Move $U_1 \cup \{v\}$ rigidly preserving heights and keeping v fixed until a distinguished edge forms with another component. Continue until the distinguished edges break the subregions into subregions with polygon boundaries. Again vor_0 and τ_0 are unchanged.

By the end of Section 4, we will deform all subregions into convex polygons.

Remark. *We will deform in such a way that the edges (v_1, v_2) will maintain a length of at least 2. The proof that distances of at least 2 are maintained is given as [HM, Lemma 7.6]. That proof uses a parameter slightly larger than 2.51, and hence it gives a result that is slightly stronger than what is needed here.*

We will deform in such a way that no vertex crosses a boundary of the subregion passing from outside to inside.

Edge length constraints prevent a vertex from crossing a boundary of the subregion from the inside to outside. In fact, if v is to cross the edge (v_1, v_2) , the simplex $S = (0, v_1, v, v_2)$ attains volume 0. We may assume, by the argument of the proof of Lemma 4.3, that there are no vertices enclosed over S . Because we are assuming that the subregion is not a triangle, we may assume that $|v - v_1| > 2.51$. We have $|v| \in [2, 2.51]$. If v is to cross (v_1, v_2) , we may assume that the dihedral angles of S along $(0, v_1)$, and $(0, v_2)$ are acute. Under these constraints, by the explicit formulas of I.8, the vertex v cannot cross out of the subregion

$$(*) \quad \Delta(S) \geq \Delta(2.51^2, 4, 4, 3.2^2, 4, 2.51^2) > 0.$$

We say that a corner v_1 is *visible* from another v_2 if (v_1, v_2) lies over the subregion. A deformation may make v_1 visible from v_2 , making it a candidate for a new distinguished edge. If $|v_1 - v_2| \leq 3.2$, then as soon as the deformation brings them into visibility (obstructed until then by some v), then $(*)$ shows that $|v_1 - v|, |v_2 - v| \leq 2.51$. So v_1, v, v_2 are consecutive edges on the polygonal boundary, and $|v_1 - v_2| \geq 2\sqrt{4 - t_0^2} > \sqrt{8}$. By the distinguished edge conditions for special simplices, (v_1, v_2) is too long to be distinguished. In other words, there can be no potentially distinguished edges hidden behind corners. They are always formed in full view.

4.9 Some deformations.

Consider three consecutive corners v_3, v_1, v_2 of a subcluster R such that the dihedral angle of R at v_1 is greater than π . We call such a corner *concave*. (If the angle is less than π , we call it *convex*.)

Let $S = S(y_1, \dots, y_6) = (0, v_1, v_2, v_3)$, $y_i = |v_i|$. Suppose that $y_6 > y_5$. Let $x_i = y_i^2$.

Lemma 4.9.1. *At a concave vertex, $\partial \text{vor}_0 / \partial x_5 > 0$ and $\partial \tau_0 / \partial x_5 < 0$.*

Proof. As x_5 varies, $\text{dih}_i(S) + \text{dih}_i(R)$ is constant for $i = 1, 2, 3$. The part of Formula F.3.7 for vor_0 that depends on x_5 can be written

$$-B(y_1) \text{dih}(S) - B(y_2) \text{dih}_2(S) - B(y_3) \text{dih}_3(S) - 4\delta_{\text{oct}}(\text{quo}(R_{135}) + \text{quo}(R_{315})),$$

where $B(y_i) = A(y_i/2) + \phi_0$, $R_{135} = R(y_1/2, b, t_0)$, $R_{315} = R(y_3/2, b, t_0)$, $b = \eta(y_1, y_3, y_5)$, and $A(h) = (1 - h/t_0)(\phi(h, t_0) - \phi_0)$. Set $u_{135} = u(x_1, x_3, x_5)$, and

$\Delta_i = \partial\Delta/\partial x_i$. (The notation comes from I.8 and F.3.) We have

$$\frac{\partial \text{quo}(R(a, b, c))}{\partial b} = \frac{-a(c^2 - b^2)^{3/2}}{3b(b^2 - a^2)^{1/2}} \leq 0$$

and $\partial b/\partial x_5 \geq 0$. Also, $u \geq 0$, $\Delta \geq 0$ (see I.8). So it is enough to show

$$V_0(S) = u_{135}\Delta^{1/2}\frac{\partial}{\partial x_5}(B(y_1)\text{dih}(S) + B(y_2)\text{dih}_2(S) + B(y_3)\text{dih}_3(S)) < 0.$$

By the explicit formulas of I.8, we have

$$V_0(S) = -B(y_1)y_1\Delta_6 + B(y_2)y_2u_{135} - B(y_3)y_3\Delta_4.$$

For τ_0 , we replace B with $B - \zeta pt$. It is enough to show that

$$V_1(S) = -(B(y_1) - \zeta pt)y_1\Delta_6 + (B(y_2) - \zeta pt)y_2u_{135} - (B(y_3) - \zeta pt)y_3\Delta_4 < 0.$$

The lemma now follows from **A**₁₄. We note that the polynomials V_i are linear in x_4 , and x_6 , and this may be used to reduce the dimension of the calculation.

□

We give a second form of the lemma when the dihedral angle of R is less than π , that is, at a convex corner.

Lemma 4.9.2. *At a convex corner, $\partial \text{vor}_0/\partial x_5 < 0$ and $\partial \tau_0/\partial x_5 > 0$, if $y_1, y_2, y_3 \in [2, 2.51]$, $\Delta \geq 0$, and (i) $y_4 \in [2\sqrt{2}, 3.2]$, $y_5, y_6 \in [2, 2.51]$, or (ii) $y_4 \geq 3.2$, $y_5, y_6 \in [2, 3.2]$.*

Proof. We adapt the proof of the previous lemma. Now $\text{dih}_i(S) - \text{dih}_i(R)$ is constant, for $i = 1, 2, 3$, so the signs change. vor_0 depends on x_5 through

$$\sum B(y_i)\text{dih}_i(S) - 4\delta_{\text{oct}}(\text{quo}(R_{135}) + \text{quo}(R_{315})).$$

So it is enough to show that

$$V_0 - 4\delta_{\text{oct}}\Delta^{1/2}u_{135}\frac{\partial}{\partial x_5}(\text{quo}(R_{135}) + \text{quo}(R_{315})) < 0.$$

Similarly, for τ_0 , it is enough to show that

$$V_1 - 4\delta_{\text{oct}}\Delta^{1/2}u_{135}\frac{\partial}{\partial x_5}(\text{quo}(R_{135}) + \text{quo}(R_{315})) < 0.$$

By **A**₁₄

$$\begin{aligned} -4\delta_{\text{oct}}u_{135}\frac{\partial}{\partial x_5}(\text{quo}(R_{135}) + \text{quo}(R_{315})) &< 0.82, \quad \text{on } [2, 2.51]^3, \\ &< 0.5, \quad \text{on } [2, 2.51]^3, y_5 \geq 2.189. \end{aligned}$$

The result now follows from the inequalities **A**₁₄. □

Return to the situation of concave corner v_1 . Let v_2, v_3 be the adjacent corners. By increasing x_5 , the vertex v_1 moves away from every corner w for which (v_1, w) lies outside the region. This deformation then satisfies the constraint of Remark 4.8. Stretch the shorter of $(v_1, v_2), (v_1, v_3)$ until $|v_1 - v_2| = |v_1 - v_3| = 3.07$ (or until a new distinguished edge forms, etc.). Do this at all concave corners.

By stopping at 3.07, we prevent a corner crossing an edge from outside-in. Let w be a corner that threatens to cross a distinguished edge (v_1, v_2) as a result of the motion at a nonconvex vertex. To say that the crossing of the edge is from the outside-in implies more precisely that the vertex being moved is an endpoint, say v_1 , of the distinguished edge. At the moment of crossing the simplex $(0, v_1, v_2, w)$ degenerates to a planar arrangement, with the projection of w lying over the geodesic arc connecting the projections of v_1 and v_2 . To see that the crossing cannot occur, it is enough to note that the volume of a simplex with opposite edges of lengths at most $2t_0$ and 3.07 and other edges at least 2 cannot be planar. The extreme case is

$$\Delta(2^2, 2^2, (2t_0)^2, 2^2, 2^2, 3.07^2) > 0.$$

If $|v_1| \geq 2.2$, we can continue the deformations even further. We stretch the shorter of (v_1, v_2) and (v_1, v_3) until $|v_1 - v_2| = |v_1 - v_3| = 3.2$ (or until a new distinguished edge forms, etc.). Do this at all concave corners v_1 for which $|v_1| \geq 2.2$. To see that corners cannot cross an edge from the outside-in, we argue as in the previous paragraph, but replacing 3.07 with 3.2. The extreme case becomes

$$\Delta(2.2^2, 2^2, (2t_0)^2, 2^2, 2^2, 3.2^2) > 0.$$

4.10 Truncated corner cells.

Because of the arguments in the Section 4.9, we may assume without loss of generality that we are working with a subregion with the following properties. If v is a concave vertex and w is not adjacent to v , and yet is visible from v , then $|v - w| \geq 3.2$. If v is a concave corner, then $|v - w| \geq 3.07$ for both adjacent corners w . If v is a concave corner and $|v| \geq 2.2$, then $|v - w| \geq 3.2$ for both adjacent corners w . These hypotheses will remain in force through the end of Section 4.

We call a spherical region convex if its interior angles are all less than π . The case where the subregion is a convex triangle will be treated in Section 5.7. Hence, we may also assume in Sections 4.10 through 4.13 that the subregion is not a convex triangle.

We construct a *corner cell* at each corner. It depends on a parameter $\lambda \in [1.6, 1.945]$. In all applications, we take $\lambda = 1.945 = 3.2 - t_0$, $\lambda = 1.815 = 3.07 - t_0$, or $\lambda = 1.6 = 3.2/2$.

To construct the cell around the corner v , place a triangle along $(0, v)$ with sides $|v|, t_0, \lambda$ (with λ opposite the origin). Generate the solid of rotation around the axis $(0, v)$. Extend to a cone over 0. Slice the solid by the perpendicular bisector of $(0, v)$, retaining the part near 0. Intersect the solid with a ball of radius t_0 . The cones over the two boundary edges of the subregion at v make two cuts in the solid. Remove the slice that lies outside the cone over the subcluster. What remains is the corner cell at v with parameter λ .

Corner cells at corners separated by a distance less than 2λ may overlap. We define a truncation of the corner cell that has the property that the *truncated corner cells* at adjacent corners do not overlap. Let $(0, v_i, v_j)^\perp$ denote the plane perpendicular to the plane $(0, v_i, v_j)$ passing through the origin and the circumcenter of $(0, v_i, v_j)$.

Let v_1, v_2, v_3 be consecutive corners of a subcluster. Take the corner cell with parameter λ at the corner v_2 . Slice it by the planes $(0, v_1, v_2)^\perp$ and $(0, v_2, v_3)^\perp$, and retain the part along the edge $(0, v_2)$. This is the truncated corner cell (tcc). By construction tccs at adjacent corners are separated by a plane $(0, \cdot, \cdot)^\perp$. Tccs at nonadjacent corners do not overlap if the corners are $\geq 2\lambda$ apart. Tccs will only be used in subregions satisfying this condition. It will be shown in Section 4.12 that tccs lie in the cone over the subregion (for suitable λ).

4.11 Formulas for Truncated corner cells.

We will assign a score to truncated corner cells, in such a way that the score of the subcluster can be estimated from the scores of the corner cells.

We write C_0 for a truncated corner cell. We write C_0^u for the corresponding untruncated corner cell. (Although we call this the untruncated corner cell to distinguish it from the corner cell, it is still truncated in the sense that it lies in the ball at the origin of radius t_0 . It is untruncated in the sense that it is not cut by the planes $(\dots)^\perp$.)

For any solid body X , we define the *geometric* truncated Voronoi function by

$$\text{vor}_0^g(X) = 4(-\delta_{oct}\text{vol}(X) + \text{sol}(X)/3)$$

the counterpart for squander

$$\tau_0^g(X) = \zeta \text{ptsol}(X) - \text{vor}_0^g(X).$$

The solid angle is to be interpreted as the solid angle of the cone formed by all rays from the origin through nonzero points of X . We may apply these definitions to obtain formulas for $\text{vor}_0^g(C_0)$, and so forth.

The formula for the score of a truncated corner cell differs slightly according to the convexity of the corner. We start with a convex corner v , and let v_1, v , and v_2 be consecutive corners in the subregion.

Let $S = (0, v, v_1, v_2)$ be a simplex with $|v_1 - v_2| \geq 3.2$. The formula for the score of a tcc $C_0(S)$ simplifies if the face of C_0 cut by $(0, v, v_1)^\perp$ does not meet the face cut by $(0, v, v_2)^\perp$. We make that assumption in this subsection. Set $\chi_0(S) = \text{vor}_0^g(C_0(S))$. (The function χ_0 is unrelated to the function χ that was introduced in Section I.8 to measure the orientation of faces.)

$$\begin{aligned} \psi &= \arccos(y_1, t_0, \lambda), \quad h = y_1/2, \\ R'_{126} &= R(y_1/2, \eta_{126}, y_1/(2 \cos \psi)), \quad R_{126} = R(y_1/2, \eta_{126}, t_0), \\ \text{sol}'(y_1, y_2, y_6) &= + \text{dih}(R'_{126})(1 - \cos \psi) - \text{sol}(R'_{126}), \\ \chi_0(S) &= \text{dih}(S)(1 - \cos \psi)\phi_0 \\ &\quad - \text{sol}'(y_1, y_2, y_6)\phi_0 - \text{sol}'(y_1, y_3, y_5)\phi_0 \\ &\quad + A(h) \text{dih}(S) - 4\delta_{oct}(\text{quo}(R_{126}) + \text{quo}(R_{135})). \end{aligned}$$

In the three lines giving the formula for χ_0 , the first line represents the score of the cone before it is cut by the planes $(0, v, v_i)^\perp$ and the perpendicular bisector of $(0, v)$. The second line is the correction resulting from cutting the tcc along the planes $(0, v, v_i)^\perp$. The face of the Rogers simplex R'_{126} lies along the plane $(0, v, v_1)^\perp$. The

third line is the correction from slicing the tcc with the perpendicular bisector of $(0, v)$. This last term is the same as the term appearing for a similar reason in the formula for vor_0 in F.3.7. In this formula R is the usual Rogers simplex and $\text{quo}(R_{ijk})$ is the quoin coming from a Rogers simplex along the face with edges (ijk) .

The formula for the untruncated corner cell is obtained by setting “sol’” and “quo” to “0” in the expression for χ_0 . Thus,

$$\text{vor}^g(C_0^u) = \text{dih}(S)[(1 - \cos \psi)\phi_0 + A(h)]$$

The formula depends only on λ , the dihedral angle, and the height $|v|$. We write $C_0^u = C_0^u(|v|, \text{dih})$, and suppress λ from the notation. The dependence on $\text{dih}(S)$ is linear:

$$\tau_0^g(C_0^u(|v|, \text{dih})) = (\text{dih}/\pi)\tau_0^g(C_0^u(|v|, \pi)).$$

The dependence of χ_0 on the fourth edge $y_4 = |v_1 - v_2|$ comes through a term proportional to $\text{dih}(S)$. Since the dihedral angle is monotonic in y_4 , so is χ_0 . Thus, under the assumption that $|v_1 - v_2| \geq 3.2$, we obtain an upper bound on χ_0 at $y_4 = 3.2$. Our deformations will fix the lengths of the other five variables, and monotonicity gives us the sixth. Thus, the tccs lead to an upper bound on vor_0^g (and a lower bound on τ_0^g) that does not require interval arithmetic.

At a concave vertex, the formula is similar. Replace “ $\text{dih}(S)$ ” with “ $(2\pi - \text{dih}(S))$ ” in the given expression for χ_0 . We add a superscript $-$ to the name of the function at concave vertices, to denote this modification: $\chi_0^-(C_0)$.

4.12 Containment of Truncated corner cells.

The assumptions made at the beginning of Section 4.10 remain in force.

Lemma 4.12.1. *Let v be a concave vertex with $|v| \geq 2.2$. The truncated corner cell at v with parameter $\lambda = 1.945$ lies in the truncated V -cell over R .*

Proof. Consider a corner cell at v and a distinguished edge (v_1, v_2) forming the boundary of the subregion. The corner cell with parameter $\lambda = 1.945$ is contained in a cone of arcradius $\theta = \text{arc}(2, t_0, \lambda) < 1.21 < \pi/2$ (in terms of the function *arc* of Section 2.8). Take two corners w_1, w_2 , visible from v , between which the given bounding edge appears. (We may have $w_i = v_i$). The two visible edges, (v, w_i) , have length ≥ 3.2 . (Recall that the distinguished edges at v have been deformed to length 3.2.) They have arc-length at least $\text{arc}(2.51, 2.51, 3.2) > 1.38$. The segment of the distinguished edge (v_1, v_2) visible from v has arc-length at most $\text{arc}(2, 2, 3.2) < 1.86$.

We check that the corner cell cannot cross the visible portion of the edge (v_1, v_2) . Consider the spherical triangle formed by the edges (v, w_1) , (v, w_2) (extended as needed) and the visible part of (v_1, v_2) . Let C be the projection of v and AB be the projection of the visible part of (v_1, v_2) . Pivot A and B toward C until the edges AC and BC have arc-length 1.38. The perpendicular from C to AB has length at least

$$\arccos(\cos(1.38)/\cos(1.86/2)) > 1.21 > \theta.$$

This proves that the corner cell lies in the cone over the subregion. \square

Lemma 4.12.2. *Let v be a concave vertex. The truncated corner cell at v with parameter $\lambda = 1.815$ lies in the truncated V -cell over R .*

Proof. The proof proceeds along the same lines as the previous lemma, with slightly different constants. Replace 1.945 with 1.815, 1.38 with 1.316, 1.21 with 1.1. Replace 3.2 with 3.07 in contexts giving a lower bound to the length of an edge at v , and keep it at 3.2 in contexts calling for an upper bound on the length of a distinguished edge. The constant 1.86 remains unchanged. \square

Lemma 4.12.3. *The truncated corner cells with parameter 1.6 in a subregion do not overlap.*

Proof. We may assume that the corners are not adjacent. If a nonadjacent corner w is visible from v , then $|w - v| \geq 3.2$, and an interior point intersection p is incompatible with the triangle inequality: $|p - v| \leq 1.6$, $|p - w| < 1.6$. If w is not visible, we have a chain $v = v_0, v_1, \dots, v_r = w$ such that v_{i+1} is visible from v_i . Imagine a taut string inside the subregion extending from v to w . The projections of v_i are the corners of the string's path. The string bends in an angle greater than π at each v_i , so the angle at each intermediate v_i is greater than π . That is, they are concave. Thus, by our deformations $|v_i - v_{i+1}| \geq 3.07$. The string has arc-length at least $r \arccos(2.51, 2.51, 3.07) > r(1.316)$. But the corner cells lie in cones of arcradius $\arccos(2, t_0, \lambda) < 1$. So $2(1.0) > r(1.316)$, or $r = 1$. Thus, w is visible from v . \square

Lemma 4.12.4. *The corner cell for $\lambda \leq 1.815$ does not overlap the t_0 -cone wedge around another corner w .*

Proof. We take $\lambda = 1.815$. As in the previous proof, if there is overlap along a chain, then

$$\arccos(2, t_0, \lambda) + \arccos(2, t_0, t_0) > r \arccos(2.51, 2.51, 3.07),$$

and again $r = 1$. So each of the two vertices in question is visible from the other. But overlap implies $|p - v| \leq 1.815$ and $|p - w| < 1.255$, forcing the contradiction $|w - v| < 3.07$. \square

Lemma 4.12.5. *The corner cell for $\lambda \leq 1.945$ at a corner v satisfying $|v| \geq 2.2$ does not overlap the t_0 -cone wedge around another corner w .*

Proof. We take $\lambda = 1.945$. As in the previous proof, if there is overlap along a chain, then

$$\arccos(2, t_0, \lambda) + \arccos(2, t_0, t_0) > r \arccos(2.51, 2.51, 3.2),$$

and again $r = 1$. Then the result follows from

$$|w - v| \leq |p - v| + |p - w| < 1.945 + 1.255 = 3.2.$$

\square

Lemma 4.3 was stated in the context of a subregion before deformation, but a cursory inspection of the proof shows that the geometric conditions required for the proof remain valid by our deformations. (This assumes that the subregion is not a triangle, which we assumed at the beginning of Section 4.10.) In more detail, there is a solid CP_0 contained in the ball of radius of t_0 at the origin, and lying over the cone of the subregion P such that a bound on the penalty-free subcluster score is $\text{vor}_0^g(CP_0)$ and squander $\tau_0^g(CP_0)$. (By *penalty-free* score, we mean the part of the

scoring bound that does not include any of the penalty terms. We will sometimes call the full score, including the penalty terms, the *penalty-inclusive* score.)

Let $\{y_1, \dots, y_r\}$ be a decomposition of the subregion into disjoint regions whose union is X . Then if we let $CP_0(y_i)$ denote the intersection of $CP_0(y_i)$ with the cone over y_i , we can write

$$\tau_0^g(CP_0) = \sum_i \tau_0^g(CP_0(y_i)).$$

These lemmas allow us to express bounds on the score (and squander) of a subcluster as a sum of terms associated with individual (truncated) corner cells. By Lemmas 4.12.1 through 4.12.5, these objects do not overlap under suitable conditions. Moreover, by the interpretation of terms provided by Section 4.3, the cones over these objects do not overlap, when the objects themselves do not. In other words, under the various conditions, we can take the (truncated) corner cells to be among the sets $CP_0(y_i)$.

To work a typical example, let us place a truncated corner cell with parameter $\lambda = 1.6$ at each concave corner. Place a t_0 -cone wedge X_0 at each convex corner. The cone over each object lies in the cone over the subregion. By Lemma 4.3 and Lemma 4.1 (see the proof), the t_0 -cone wedge X_0 squanders a positive amount. The part P' of the subregion outside all truncated corner cells and outside the t_0 -cone wedges squanders

$$\text{sol}(P')(\zeta pt - \phi_0) > 0.$$

where $\text{sol}(P')$ is the part of the solid angle of the subregion lying outside the tcgs. Dropping these positive terms, we obtain a lower bound on the penalty-free squander:

$$\tau_0^g(CP_0) \geq \sum_{C_0} \tau_0^g(C_0).$$

There is one summand for each concave corner of the subregion. Other cases proceed similarly.

4.13 Convexity.

Lemma 4.13.1. *There are at most two concave corners.*

Proof. Use the parameter $\lambda = 1.6$ and place a truncated corner cell C_0 at each concave corner v . Let $C_0^u(|v|, \text{dih})$ denote the corresponding untruncated cell. Formula 4.11 gives

$$\tau_0^g(C_0) = \tau_0^g(C_0^u(|v|, \text{dih})) - \text{sol}'(y_1, y_2, y_6)\phi'_0 - \text{sol}'(y_1, y_3, y_5)\phi'_0,$$

where $\phi'_0 = \zeta pt - \phi_0 < 0.6671$. (The conditions $y_5 \geq 3.07$ and $y_6 \geq 3.07$ force the faces along these edges to have circumradius greater than t_0 , and this causes the “quo” terms in the formula to be zero.)

By monotonicity in dih , a lower bound on $\tau_0^g(C_0^u)$ is obtained at $\text{dih} = \pi$. $\tau_0(C_0^u(|v|, \pi))$ is an explicit monotone decreasing rational function of $|v| \in [2, 2.51]$, which is minimized for $|v| = 2.51$. We find

$$\tau_0(C_0^u(|v|, \text{dih})) \geq \tau_0(C_0^u(2.51, \pi)) > 0.32.$$

The term $\text{sol}'(y_1, y_3, y_5)$ is maximized when $y_3 = 2.51$, $y_5 = 3.07$, so that $\text{sol}' < 0.017$. (This was checked with interval arithmetic in Mathematica.) Thus,

$$\tau_0(C_0(v)) \geq 0.32 - 2(0.017)\phi'_0 > 0.297.$$

If there are three or more concave corners, then the penalty-free corner cells squander at least $3(0.297)$. The penalty is at most π_{\max} (Section 4.7). So the penalty-inclusive squander is more than $3(0.297) - \pi_{\max} > (4\pi\zeta - 8)pt$. \square

Lemma 4.13.2. *There are no concave corners of height at most 2.2.*

Proof. Suppose there is a corner of height at most 2.2. Place an untruncated corner cell $C_0^u(|v|, \text{dih})$ with parameter $\lambda = 1.815$ at that corner and a t_0 -cone wedge at every other corner. The subcluster squanders at least $\tau_0(C_0(|v|, \pi)) - \pi_{\max}$. This is an explicit monotone decreasing rational function of one variable. The penalty-inclusive squander is at least

$$\tau_0(C_0^u(2.51, \pi)) - \pi_{\max} > (4\pi\zeta - 8)pt.$$

\square

By the assumptions at the beginning of Section 4.10, the lemma implies that each concave corner has distance at least 3.2 from every other visible corner.

As in the previous lemma, when $\lambda = 1.945$, a lower bound on what is squandered by the corner cell is obtained for $|v| = 2.51$, $\text{dih} = \pi$. The explicit formulas give penalty-free squander > 0.734 . Two disjoint corner cells give penalty-inclusive squander $> (4\pi\zeta - 8)pt$. Suppose two at v_1, v_2 overlap. The lowest bound is obtained when $|v_1 - v_2| = 3.2$, the shortest distance possible.

We define a function $f(y_1, y_2)$ that measures what the union of the overlapping corner cells squander. Set $y_i = |v_i|$, $\ell = 3.2$, and

$$\begin{aligned} \alpha_1 &= \text{dih}(y_1, t_0, y_2, \lambda, \ell, \lambda), \\ \alpha_2 &= \text{dih}(y_2, t_0, y_1, \lambda, \ell, \lambda), \\ \text{sol} &= \text{sol}(y_2, t_0, y_1, \lambda, \ell, \lambda), \\ \phi_i &= \phi(y_i/2, t_0), \quad i = 1, 2, \\ \lambda &= 3.2 - t_0 = 1.945, \end{aligned}$$

$$\begin{aligned} f(y_1, y_2) &= 2(\zeta pt - \phi_0) \text{sol} + 2 \sum_{i=1}^2 \alpha_i (1 - y_i/(2t_0)) (\phi_0 - \phi_i) \\ &\quad + \sum_{i=1}^2 \tau_0(C(y_i, \lambda, \pi - 2\alpha_i)). \end{aligned}$$

\mathbf{A}_{14} gives $f(y_1, y_2) > (4\pi\zeta - 8)pt + \pi_{\max}$, for $y_1, y_2 \in [2, 2.51]$.

We conclude that there is at most one concave corner. Let v be such a corner. If we push v toward the origin, the solid angle is unchanged and vor_0 is increased. Following this by the deformation of Section 4.9, we maintain the constraints $|v - w| = 3.2$, for adjacent corners w , while moving v toward the origin. Eventually $|v| = 2.2$. This is impossible by Lemma 4.13.2.

We verify that this deformation preserves the constraint $|v - w| \geq 2$, for all corners w such that (v, w) lies entirely outside the subregion. In fact, every corner is visible from v , so that the subregion is star convex at v . We leave the details to the reader.

We conclude that all subregions can be deformed into convex polygons.

5. CONVEX POLYGONS

5.1 Deformations. We divide the bounding edges over the polygon according to length $[2, 2.51]$, $[2.51, 2\sqrt{2}]$, $[2\sqrt{2}, 3.2]$. The deformations of Section 4.9 contract edges to the lower bound of the intervals (2, 2.51, or $2\sqrt{2}$) unless a new distinguished edge is formed. By deforming the polygon, we assume that the bounding edges have length 2, 2.51, or $2\sqrt{2}$. (There are a few instances of triangles or quadrilaterals that do not satisfy the hypotheses needed for the deformations. These instances will be treated in Sections 5.7 and 5.8.)

Lemma 5.1.1. *Let $S = S(y_1, \dots, y_6)$ be a simplex, with $x_i = y_i^2$, as usual. Let $y_4 \geq 2$, $\Delta \geq 0$, $y_5, y_6 \in \{2, 2.51, 2\sqrt{2}\}$. Fixing all the variables but x_1 , let $f(x_1)$ be one of the functions $\text{vor}_0(S)$ or $-\tau_0(S)$. We have $f''(x_1) > 0$ whenever $f'(x_1) = 0$.*

Proof. This is an interval calculation **A**₁₅. \square

The lemma implies that f does not have an interior point local maximum for $x_1 \in [2^2, 2.51^2]$. Fix three consecutive corners, v_0, v_1, v_2 of the convex polygon, and apply the lemma to the variable $x_1 = |v_1|^2$ of the simplex $S = (0, v_0, v_1, v_2)$. We deform the simplex, increasing f . If the deformation produces $\Delta(S) = 0$, then some dihedral angle is π , and the arguments for nonconvex regions bring us eventually back to the convex situation. Eventually y_1 is 2 or 2.51. Applying the lemma at each corner, we may assume that the height of every corner is 2 or 2.51. (There are a few cases where the hypotheses of the lemma are not met, and these are discussed in Sections 5.7 and 5.8.)

Lemma 5.1.2. *The convex polygon has at most 7 sides.*

Proof. Since the polygon is convex, its perimeter on the unit sphere is at most a great circle 2π . If there are 8 sides, the perimeter is at least $8 \arccos(2.51/2) > 2\pi$. \square

5.2 Truncated corner cells.

The following lemma justifies using tcCs at the corners as an upper bound on the score (and lower bound on what is squandered). We fix the truncation parameter at $\lambda = 1.6$.

Lemma. *Take a convex subregion that is not a triangle. Assume edges between adjacent corners have lengths $\in \{2, 2.51, 2\sqrt{2}, 3.2\}$. Assume nonadjacent corners are separated by distances ≥ 3.2 . Then the truncated corner cell at each vertex lies in the cone over the subregion.*

Proof. Place a tcc at v_1 . For a contradiction, let (v_2, v_3) be an edge that the tcc overlaps. Assume first that $|v_1 - v_i| \geq 2.51$, $i = 2, 3$. Pivot so that $|v_1 - v_2| = |v_1 - v_3| = 2.51$. Write $S(y_1, \dots, y_6) = (0, v_1, v_2, v_3)$. Set $\psi = \arccos(y_1, t_0, 1.6)$. **A**₁ gives $\beta_\psi(y_1, y_2, y_6) < \text{dih}_2(S)$.

Now assume $|v_1 - v_2| < 2.51$. By the hypotheses of the lemma, $|v_1 - v_2| = 2$. If $|v_1 - v_3| < 3.2$, then $(0, v_1, v_2, v_3)$ is triangular, contrary to hypothesis. So $|v_1 - v_3| \geq 3.2$. Pivot so that $|v_1 - v_3| = 3.2$. By **A**₁,

$$\beta_\psi(y_1, y_2, y_6) < \text{dih}_2(S),$$

where $\psi = \arccos(y_1, t_0, 1.6)$, provided $y_1 \in [2.2, 2.51]$. Also, if $y_1 \in [2.2, 2.51]$

$$\arccos(y_1, t_0, 1.6) < \arccos(y_1, y_2, y_6).$$

If $y_1 \leq 2.2$, then $\Delta_1 \geq 0$, so $\partial \text{dih}_2 / \partial x_3 \leq 0$. Set $x_3 = 2.51^2$. Also, $\Delta_6 \geq 0$, so $\partial \text{dih}_2 / \partial x_4 \leq 0$. Set $x_4 = 3.2^2$.

Let c be a point of intersection of the plane $(0, v_1, v_2)^\perp$ with the circle at distance $\lambda = 1.6$ from v_1 on the sphere centered at the origin of radius t_0 . The angle along $(0, v_2)$ between the planes $(0, v_2, v_1)$ and $(0, v_2, c)$ is

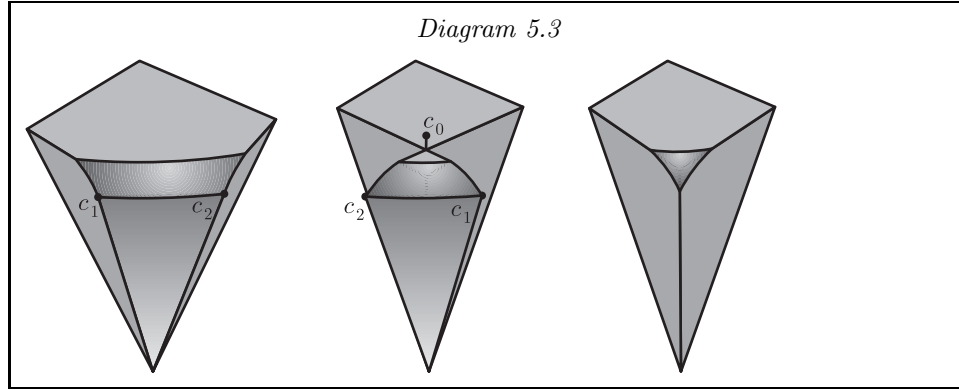
$$\text{dih}(R(y_2/2, \eta_{126}, y_1/(2 \cos \psi))).$$

This angle is less than $\text{dih}_2(S)$ by **A₁**. Also, $\Delta_1 \geq 0$, $\partial \text{dih}_3 / \partial x_2 \leq 0$, so set $x_2 = 2.51^2$. Then $\Delta_5 < 0$, so $\text{dih}_2 > \pi/2$. This means that $(0, v_1, v_2)^\perp$ separates the tcc from the edge (v_2, v_3) . \square

5.3 Analytic continuation.

In this subsection we assume that $\lambda = 1.6$ and that the truncated corner cell under consideration lies at a convex vertex.

Assume that the face cut by $(0, v, v_1)^\perp$ meets the face cut by $(0, v, v_2)^\perp$. Let c_i be the point on the plane $(0, v, v_i)^\perp$ satisfying $|c_i - v| = 1.6$, $|c_i| = t_0$. (Pick the root within the wedge between v_1 and v_2 .) The overlap of the two faces is represented in the diagram.



We let c_0 be the point of height $t_0 = 1.255$ on the intersection of the planes $(0, v, v_1)^\perp$ and $(0, v, v_2)^\perp$. We claim that c_0 lies over the truncated spherical region of the tcc, rather than the wedges of t_0 -cones or the Rogers simplices along the faces $(0, v, v_1)$ and $(0, v, v_2)$. (This implies that c_0 cannot protrude beyond the corner cell as depicted in the second frame of the diagram.) To see the claim, consider the tcc as a function of $y_4 = |v_1 - v_2|$. When y_4 is sufficiently large the claim is certainly true. Contract y_4 until $c_0 = c_0(y_4)$ meets the perpendicular bisector of $(0, v)$. Then c_0 is equidistant from $0, v, v_1$ and v_2 so it is the circumcenter of $(0, v, v_1, v_2)$. It has distance t_0 from the origin, so the circumradius is t_0 . This implies that $y_4 \leq 2.51$.

The tcc is defined by the constraints represented in the third frame. The analytic continuation of the function $\chi_0(S) = \chi_0^{\text{an}}(S)$, defined above, acquires a volume X , counted with negative sign, lying under the spherical triangle (c_0, c_1, c_2) . Extending our notation, we have an analytically defined function χ_0^{an} and a geometrically defined function χ_0^g ,

$$\begin{aligned} \chi_0^{\text{an}}(S) &= \chi_0^g(S) - \text{vor}_0(X), \text{ where} \\ \text{vor}_0(X) &= 4(-\delta_{\text{oct}} \text{vol}(X) + \text{sol}(X)/3) = \phi_0 \text{sol}(X) < 0. \end{aligned}$$

So $\chi_0^{\text{an}} > \chi_0^g$, and we may always use $\chi_0(S) = \chi_0^{\text{an}}(S)$ as an upper bound on the score of a tcc.

For example, with $\lambda = 1.6$ and $S = S(2.3, 2.3, 2.3, 2.9, 2, 2)$, we have

$$\chi_0^{\text{an}}(S) \approx -0.103981, \quad \chi_0^g(S) \approx -0.105102.$$

Or, if $S = S(2, 2, 2.51, 3.2, 2, 2.51)$, then

$$\chi_0^{\text{an}}(S) \approx -0.0718957, \quad \chi_0^g(S) \approx -0.0726143.$$

5.4 Penalties.

In Section 4.7, we determined the bound of $\pi_{\max} = 0.06688$ on penalties. In this section, we give a more thorough treatment of penalties. Until now a penalty has been associated with a given standard region, but by taking the worst case on each subregion, we can move the penalties to the level of subregions. Roughly, each subregion should incur the penalties from the upright quarters that were erased along edges of that subregion. Each upright quarter of the original standard region is attached at an edge between adjacent corners of the standard cluster. The edges have lengths between 2 and 2.51. The deformations shrink the edges to length 2. We attach the penalty from the upright quarter to this edge of this subregion. In general, we divide the penalty evenly among the upright quarters along a common diagonal, without trying to determine a more detailed accounting. For example, the penalty 0.008 in Section 3.9 comes from three upright quarters. Thus, we give each of three edges a penalty of $0.008/3$. Or, if there are only two upright quarters in the group \mathbf{S}_3^+ , then each of the two upright quarters is assigned the penalty $0.00222/2$ (see Lemma 3.9.2).

The penalty $0.04683 = 3\xi_\Gamma$ in Section 4.7 comes from three upright quarters \mathbf{S}_3^- . Each of three edges is assigned a penalty of ξ_Γ . The penalty $0.03344 = 3\xi_\Gamma + \xi_{\kappa,\Gamma}$ comes from the arrangement of four upright quarters \mathbf{S}_4^+ of Section 3.8. It is divided among 4 edges. These are the only upright quarters that take a penalty when erased. (The case of two upright quarters over a flat quarter as in Lemma 3.4, are treated by a separate argument in Section 5.7. Loops will be discussed in Section 5.11.)

The penalty can be reduced in various situations involving a masked flat quarter. For example, in the three-quarter configuration \mathbf{S}_3^- , if there is a masked flat quarter, two of the uprights are scored by the analytic Voronoi function, so that the penalty plus adjustment is only $0.034052 = 2\xi_V + \xi_\Gamma + 0.0114$ (by $\mathbf{A}_{10}, \mathbf{A}_{11}$). The adjustment 0.0114 reflects the scoring rules for masked flat quarters (Section 3.9). This we divide evenly among the three edges that carried the upright quarters. If e is an edge of the subregion R , let $\pi_0(R, e)$ denote the penalty and score adjustment along edge e of R .

In summary, we have the penalties,

$$\xi_\kappa, \xi_V, \xi_\Gamma, \quad 0.008,$$

combined in various ways in the configurations $\mathbf{S}_3^-, \mathbf{S}_3^+, \mathbf{S}_4^+$. There are score adjustments

$$0.0114 \quad \text{and} \quad 0.0063$$

from Section 3.10 for masked flat quarters. If the sum of these contributions is s , we set $\pi_0(R, e) = s/n$, for each edge e of R originating from an erased upright quarter of \mathbf{S}_n^\pm .

5.5 Penalties and Bounds.

Recall that the bounds for flat quarters we wish to establish from Section 4.5 are $Z(3, 1) = 0.00005$ and $D(3, 1) = 0.06585$. Flat quarters arise in two different ways. Some flat quarters are present before the deformations begin. They are scored by the rules of Section 3.10. Others are formed by the deformations. In this case, they are scored by vor_0 . Since the flat quarter is broken away from the subregion as soon as the diagonal reaches $2\sqrt{2}$, and then is not deformed further, the diagonal is fixed at $2\sqrt{2}$. Such flat quarters can violate our desired inequalities. For example,

$$Z(3, 1) < \text{vor}_0(S(2, 2, 2, 2\sqrt{2}, 2, 2)) \approx 0.00898, \quad \tau_0(S(2, 2, 2, 2\sqrt{2}, 2, 2)) \approx 0.0593.$$

On the other hand, as we will see, the adjacent subregion satisfies the inequality by a comfortable margin. Therefore, we define a transfer ϵ from flat quarters to the adjacent subregion. (In an exceptional region, the subregion next to a flat quarter along the diagonal is not a flat quarter.)

For a flat quarter Q , set

$$\begin{aligned} \epsilon_\tau(Q) &= \begin{cases} 0.0066, & \text{(deformation),} \\ 0, & \text{(otherwise).} \end{cases} \\ \epsilon_\sigma(Q) &= \begin{cases} 0.009, & \text{(deformation),} \\ 0, & \text{(otherwise).} \end{cases} \end{aligned}$$

The nonzero value occurs when the flat quarter Q is obtained by deformation from an initial configuration in which Q is not a quarter. The value is zero when the flat quarter Q appears already in the undeformed standard cluster. Set

$$\begin{aligned} \pi_\tau(R) &= \sum_e \pi_0(R, e) + \sum_e \pi_0(Q, e) + \sum_Q \epsilon_\tau(Q), \\ \pi_\sigma(R) &= \sum_e \pi_0(R, e) + \sum_e \pi_0(Q, e) + \sum_Q \epsilon_\sigma(Q). \end{aligned}$$

The first sum runs over the edges of a subregion R . The second sum runs over the edges of the flat quarters Q that lie adjacent to R along the diagonal of Q .

The edges between corners of the polygon have lengths 2, 2.51, or $2\sqrt{2}$. Let k_0 , k_1 , and k_2 be the number of edges of these three lengths respectively. By Lemma 5.1, we have $k_0 + k_1 + k_2 \leq 7$. Let $\tilde{\sigma}$ denote any of the functions of Section 3.10.(a)–(f). Let $\tilde{\tau} = \text{sol } \zeta pt - \tilde{\sigma}$.

To prove Theorem 4.4, refining the strategy proposed in Section 4.5, we must show that for each flat quarter Q and each subregion R that is not a flat quarter, we have

$$\begin{aligned} \tilde{\tau}(Q) &> D(3, 1) - \epsilon_\tau(Q), \\ \tau_0(Q) &> D(3, 1) - \epsilon_\tau(Q), \quad \text{if } y_4(Q) = 2\sqrt{2}, \\ \tau_V(R) &> D(3, 2), \quad (\text{type } S_A), \\ (5.5.1) \quad \tau_0(R) &> D(k_0 + k_1 + k_2, k_1 + k_2) + \pi_\tau(R), \end{aligned}$$

where $D(n, k)$ is the function defined in Section 4.5. The first of these inequalities follows from $\mathbf{A}_1, \mathbf{A}_{13}, \mathbf{A}_{16}$. In general, we are given a subregion without explicit information about what the adjacent subregions are. Similarly, we have discarded all information about what upright quarters have been erased. Because of this, we assume the worst, and use the largest feasible values of π_τ .

Lemma. *We have $\pi_\tau(R) \leq 0.04683 + (k_0 + 2k_2 - 3)0.008/3 + 0.0066k_2$.*

Proof. The worst penalty $0.04683 = 3\xi_\Gamma$ per edge comes from \mathbf{S}_3^- . The number of penalized edges not on \mathbf{S}_3^- is at most $k_0 + 2k_2 - 3$. For every three edges we might have one \mathbf{S}_3^+ . The other cases such as \mathbf{S}_4^+ or situations with a masked flat quarter are readily seen to give smaller penalties. \square

For bounds on the score, the situation is similar. The only penalties we need to consider are 0.008 from Section 3.9. If either of the other configurations of upright quarters $\mathbf{S}_3^-, \mathbf{S}_4^+$ occur, then the score of the standard cluster is less than $s_8 = -0.228$, by Sections 3.7 and 3.8. This is the desired bound. So it is enough to consider subregions that do not have these upright configurations. Moreover, the penalty 0.008 does not occur in connection with masked flats. So we can take $\pi_\sigma(R)$ to be

$$(k_0 + 2k_2)0.008/3 + 0.009k_2.$$

If $k_0 + 2k_2 < 3$, we can strengthen this to $\pi_\sigma(R) = 0.009k_2$. Let $\tilde{\sigma}$ be any of the functions of Section 3.10.(a)–(f). To prove Theorem 4.4, we will show

$$\begin{aligned} \tilde{\sigma}(Q) &< Z(3, 1) + \epsilon_\sigma(Q), \\ \text{vor}_0(Q) &< Z(3, 1) + \epsilon_\sigma(Q), \quad \text{if } y_4(Q) = 2\sqrt{2}, \\ \text{vor}_0(R) &< Z(3, 2), \quad (\text{type } S_A), \\ (5.5.2) \quad \text{vor}_0(R) &< Z(k_0 + k_1 + k_2, k_1 + k_2) - \pi_\sigma(R). \end{aligned}$$

The first of these inequalities follows from $\mathbf{A}_1, \mathbf{A}_{13}, \mathbf{A}_{16}$.

5.6 Constants.

Theorem 4.4 now results from the calculation of a host of constants. Perhaps there are simpler ways to do it, but it was a routine matter to run through the long list of constants by computer. What must be checked is that the Inequalities 5.5.1 and 5.5.2 hold for all possible convex subregions. This section describes in detail the constants to check.

We begin with a subregion given as a convex n -gon, with at least 4 sides. The heights of the corners and the lengths of edges between adjacent edges have been reduced by deformation to a finite number of possibilities (lengths 2, 2.51, or lengths 2, 2.51, $2\sqrt{2}$, respectively). By Lemma 5.1, we may take $n = 4, 5, 6, 7$. Not all possible assignments of lengths correspond to a geometrically viable configuration. One constraint that eliminates many possibilities, especially heptagons, is that of Section 5.1: the perimeter of the convex polygon is at most a great circle. Eliminate all length-combinations that do not satisfy this condition. When there is a special simplex it can be broken from the subregion and scored separately unless the two heights along the diagonal are 2 (see \mathbf{A}_{13}). We assume in all that follows that all specials that can be broken off have been. There is a second condition related to special simplices. We have $\Delta(2.51^2, 2^2, 2^2, x^2, 2^2, 2^2) < 0$, if $x > 3.114467$. This means that if the cluster edges along the polygon are $(y_1, y_2, y_3, y_5, y_6) = (2.51, 2, 2, 2, 2)$, the simplex must be special ($y_4 \in [2\sqrt{2}, 3.2]$).

The easiest cases to check are those with no special simplices over the polygon. In other words, these are subregions for which the distances between nonadjacent corners are at least 3.2. In this case we approximate the score (and what is squandered) by t_{ccs} at the corners. We use monotonicity to bring the fourth edge to

length 3.2. We calculate the tcc constant bounding the score, checking that it is less than the constant $Z(k_0 + k_1 + k_2, k_1 + k_2) - \pi_\sigma$, from (5.5.2). The bounds for τ_0 are verified in the same way.

When $n = 5, 6, 7$, and there is one special simplex, the situation is not much more difficult. By our deformations, we decrease the lengths of edges 2, 3, 5, 6 of the special to 2. We remove the special by cutting along its fourth edge e (the diagonal). We score the special with the weak bounds found in \mathbf{A}_{13} . Along the edge e , we then apply deformations to the $(n - 1)$ -gon that remains. If this deformation brings e to length $2\sqrt{2}$, then the $(n - 1)$ -gon may be scored with tccs as in the previous paragraph. But there are other possibilities. Before e drops to $2\sqrt{2}$, a new distinguished edge of length 3.2 may form between two corners (one of the corners will be a chosen endpoint of e). The subregion breaks in two. By deformations, we eventually arrive at $e = 2\sqrt{2}$ and a subregion with diagonals of length at least 3.2. (There is one case that may fail to be deformable to $e = 2\sqrt{2}$, a pentagonal cases discussed further in Section 5.9.) The process terminates because the number of sides to the polygon drops at every step. A simple recursive computer procedure runs through all possible ways the subregion might break into pieces and checks that the tcc-bound gives Inequalities (5.5.1) and (5.5.2). The same argument works if there is a special simplex that overlaps each of the other special simplices in the subcluster.

When $n = 6, 7$ and there are two nonoverlapping special simplices, a similar argument can be applied. Remove both specials by cutting along the diagonals. Then deform both diagonals to length $2\sqrt{2}$, taking into account the possible ways that the subregion can break into pieces in the process. In every case the bounds (5.5.1) and (5.5.2) are satisfied.

There are a number of situations that arise that escape this generic argument and were analyzed individually. These include the cases involving more than two special simplices over a given subregion, two special simplices over a pentagon, or a special simplex over a quadrilateral. Also, the deformation lemmas are insufficient to bring all of the edges between adjacent corners to one of the three standard lengths 2, 2.51, $2\sqrt{2}$ for certain triangular and quadrilateral regions. These are treated individually.

The next few sections describe the cases treated individually. The cases not mentioned in the sections that follow fall within the generic procedure just described.

5.7 Triangles.

With triangular subregions, there is no need to use any of the deformation arguments because the dimension is already sufficiently small to apply interval arithmetic directly to obtain our bounds. There is no need for the tcc-bound approximations.

Flat quarters and simplices of type S_A are treated in \mathbf{A}_{16} . Other simplices are scored by the truncated Voronoi function. We break the edges between corners into the cases $[2, 2.51)$, $[2.51, 2\sqrt{2})$, $[2\sqrt{2}, 3.2]$. Let k_0 , k_1 , and k_2 , with $k_0 + k_1 + k_2 = 3$, be the number of edges in the respective intervals.

If $k_2 = 0$, we can improve the penalties,

$$\pi_\tau = \pi_\sigma = 0.$$

To see this, first we observe that there can be no \mathbf{S}_3^- or \mathbf{S}_4^+ configurations. By placing ≥ 3 quarters around an upright diagonal, if the subregion is triangular, the

upright diagonal becomes surrounded by anchored simplices, a case deferred until Section 5.11.

If $k_0 = k_1 = k_2 = 1$, we can take $\pi'_\tau = \xi_\Gamma + 2\xi_V + 0.0114 = 0.034052$. A few cases are needed to justify this constant. If there are no \mathbf{S}_3^- configurations, π'_τ is at most

$$\begin{aligned} & [\xi_\Gamma + 2\xi_V + \xi_{\kappa,\Gamma}]3/4 < 0.0254, \\ \text{or } & [\xi_\Gamma + 2\xi_V + \xi_{\kappa,\Gamma}]2/4 + 0.008/3 < 0.0254 \end{aligned}$$

If there are at most two edges in the subregion coming from an \mathbf{S}_3^- configuration,

$$(\xi_\Gamma + 2\xi_V + 0.0114)2/3 + 0.008/3 < 0.0254.$$

If three edges come from an \mathbf{S}_3^- configuration, we get 0.034052. To get somewhat sharper bounds, we consider how the edge k_2 was formed. If it is obtained by deformation from an edge in the standard region of length ≥ 3.2 , then it becomes a distinguished edge when the length drops to 3.2. If the edge in the standard region already has length ≤ 3.2 , then it is distinguished before the deformation process begins, so that the subregion can be treated in isolation from the other subregions. We conclude that when $\pi'_\tau = 0.034052$ we can take $y_4 \geq 2.6$ or $y_5 = 3.2$ (Remark 3.9).

The bounds (5.5.1) and (5.5.2) now follow from \mathbf{A}_{17} and \mathbf{A}_{18} .

5.8 Quadrilaterals.

We introduce some notation for the heights and edge lengths of a convex polygon. The heights will generally be 2 or 2.51, the edge lengths between consecutive corners will generally be 2, 2.51, or $2\sqrt{2}$. We represent the edge lengths by a vector

$$(a_1, b_1, a_2, b_2, \dots, a_n, b_n),$$

if the corners of an n -gon, ordered cyclically have heights a_i and if the edge length between corner i and $i + 1$ is b_i . We say two vectors are equivalent if they are related by a different cyclic ordering on the corners of the polygon, that is, by the action of the dihedral group.

The vector of a polygon with a special simplex is equivalent to one of the form $(2, 2, a_2, 2, 2, \dots)$. If $a_2 = 2.51$, then what we have is necessarily special (Section 5.6). However, if $a_2 = 2$, it is possible for the edge opposite a_2 to have length greater than 3.2.

Turning to quadrilateral regions, we use tcc scoring if both diagonals are greater than 3.2. Suppose that both diagonals are between $[2\sqrt{2}, 3.2]$, creating a pair of overlapping special simplices. The deformation lemma requires a diagonal longer than 3.2, so although we can bring the quadrilateral to the form

$$(a_1, 2, 2, 2, 2, 2, a_4, b_4),$$

the edges a_1, a_4, b_4 and the diagonal vary continuously (see \mathbf{A}_{13}). By \mathbf{A}_{19} , we have bounds on the score

$$\begin{aligned} \tau_0 &> 0.235, \quad \text{vor}_0 < -0.075, \text{ if } b_4 \in [2.51, 2\sqrt{2}], \\ \tau_0 &> 0.3109, \quad \text{vor}_0 < -0.137, \text{ if } b_4 \in [2\sqrt{2}, 3.2], \end{aligned}$$

We have $D(4, 1) = 0.2052$, $Z(4, 1) = -0.05705$. When $b_4 \in [2.51, 2\sqrt{2}]$, we can take $\pi_\tau = \pi_\sigma = 0$. (We are excluding loops here.) When $b_4 \in [2\sqrt{2}, 3.2]$, we can take

$$\begin{aligned}\pi_\tau &= \pi_{\max} + 0.0066, \\ \pi_\sigma &= 0.008(5/3) + 0.009.\end{aligned}$$

It follows that the Inequalities (5.5.1) and (5.5.2) are satisfied.

Suppose that one diagonal has length $[2\sqrt{2}, 3.2]$ and the other has length at least 3.2. The quadrilateral is represented by the vector

$$(2, 2, a_2, 2, 2, b_3, a_4, b_4).$$

The hypotheses of the deformation lemma hold, so that $a_i \in \{2, 2.51\}$ and $b_j \in \{2, 2.51, 2\sqrt{2}\}$. To avoid quad clusters, we assume $b_4 \geq \max(b_3, 2.51)$. These are one-dimensional with a diagonal of length $[2\sqrt{2}, 3.2]$ as parameter. The required verifications appear in \mathbf{A}_{20} .

5.9 Pentagons.

Some extra comments are needed when there is a special simplex. The general argument outlined above removes the special, leaving a quadrilateral. The quadrilateral is deformed, bringing the edge that was the diagonal of the special to $2\sqrt{2}$. This section discusses how this argument might break down.

Suppose first that there is a special and that both diagonals on the resulting quadrilateral are at least 3.2. We can deform using either diagonal, keeping both diagonals at least 3.2. The argument breaks down if both diagonals drop to 3.2 before the edge of the special reaches $2\sqrt{2}$ and both diagonals of the quadrilateral lie on specials. When this happens, the quadrilateral has the form

$$(2, 2, 2, 2, 2, 2, 2, b_4),$$

where b_4 is the edge originally on the special simplex. If both diagonals are 3.2, this is rigid, with $b_4 = 3.12$. We find its score to be

$$\begin{aligned}\text{vor}_0(S(2, 2, 2, b_4, 3.2, 2)) + \text{vor}_0(S(2, 2, 2, 3.2, 2, 2)) + 0.0461 &< -0.205, \\ \tau_0(S(2, 2, 2, b_4, 3.2, 2)) + \tau_0(S(2, 2, 2, 3.2, 2, 2))2 &> 0.4645.\end{aligned}$$

So the Inequalities (5.5.1) and (5.5.2) hold easily.

If there is a special and there is a diagonal on resulting quadrilateral ≤ 3.2 , we have two nonoverlapping specials. It has the form

$$(2, 2, a_2, 2, 2, 2, a_4, 2, 2, b_5).$$

The edges a_2 and a_4 lie on the special. If $b_5 > 2$, cut away one of the special simplices. What is left can be reduced to a triangle, or a quadrilateral case treated in \mathbf{A}_{20} . Assume $b_5 = 2$. We have a pentagonal standard region. We may assume that there is no \mathbf{S}_4^+ or \mathbf{S}_3^- configuration, for otherwise Theorem 4.4 follows trivially from the bounds in Section 2. A pentagon can then have at most \mathbf{S}_3^+ for a penalty of 0.008.

If $a_2 = 2.51$ or $a_4 = 2.51$, we again remove a special simplex and produce triangles, quadrilaterals, or the special cases in \mathbf{A}_{20} . We may impose the condition $a_2 = a_4 = b_5 = 2$. We score this full pentagonal arrangement in \mathbf{A}_{21} , using the edge lengths of the two diagonals of the specials as variables. The inequalities follow.

5.10 Hexagons and heptagons.

We turn to hexagons. There may be three specials whose diagonals do not cross. Such a subcluster is represented by the vector

$$(2, 2, a_2, 2, 2, 2, a_4, 2, 2, 2, a_6, 2).$$

The heights a_{2i} are 2 or 2.51. Draw the diagonals between corners 1, 3, and 5. This is a three-dimensional configuration, determined by the lengths of the three diagonals. The required bound follows from \mathbf{A}_{21} .

There is one case with a special simplex that did not satisfy the generic computer-checked inequalities for what is to be squandered. Its vector is

$$(a_1, 2, 2, 2, 2, 2, 2, b_4, 2, 2, 2, 2),$$

with $a_1 = b_4 = 2.51$. A vertex of the special simplex has height $a_1 = 2.51$ and all other corners have height 2. The subregion is a hexagon with one edge longer than 2. We have $D(6, 1) = 0.48414$. This is certainly obtained if the subregion contains the configuration \mathbf{S}_3^- squandering 0.5606. But if this configuration does not appear, we can decrease π_τ to $0.03344 + (2/3)0.008$, a constant coming from \mathbf{S}_4^+ in Section 4.7. With this smaller penalty the inequality is satisfied.

Now turn to heptagons. The bound 2π on the perimeter of the polygon, eliminates all but one equivalence class of vectors associated with a polygon that has two or more potentially specials simplices. The vector is

$$(2, 2, a_2, 2, 2, 2, a_4, 2, 2, 2, a_6, 2, a_7, 2),$$

$a_2 = a_4 = a_6 = a_7 = 2.51$. In other words, the edges between adjacent corners are 2 and four heights are 2.51. There are two specials. This case is treated by the procedure outlined for subregions with two specials whose diagonals do not cross.

5.11 Loops.

We now return to a collection of anchored simplices that surround the upright diagonal. This is the last case needed to complete the proof of Theorem 4.5. There are four or five anchored simplices around the upright diagonal. \mathbf{A}_2 – \mathbf{A}_7 give a list of linear inequalities satisfied by the anchored simplices, broken up according to type: upright, type S_C , opposite edge > 3.2 , etc. The anchored simplices are related by the constraint that the sum of the dihedral angles around the upright diagonal is 2π . We run a linear program in each case based on these linear inequalities, subject to this constraint to obtain bounds on the score and what is squandered by the anchored simplices.

When the edge opposite the diagonal of an anchored simplex has length $\in [2\sqrt{2}, 3.2]$ and the simplex adjacent to the anchored simplex across that edge is a special simplex, we use the inequalities \mathbf{A}_{22} and \mathbf{A}_{23} that run parallel to \mathbf{A}_4 and \mathbf{A}_5 . It is not necessary to run separate linear programs for these. It is enough to observe that the constants for what is squandered improve on those from \mathbf{A}_4 by at least 0.06445 and that the constants for the score in \mathbf{A}_{22} differ with those of \mathbf{A}_4 by no more than 0.009.

When the dihedral angle of an anchored simplex is greater than 2.46, the simplex is dropped, and the remaining anchored simplices are subject to the constraint that their dihedral angles sum to at most $2\pi - 2.46$. There can not be an anchored

simplex with dihedral angle greater than 2.46 when there are five anchors: $2.46 + 4(0.956) > 2\pi$. There cannot be two anchored simplices with dihedral angle greater than 2.46: $2(2.46 + 0.956) > 2\pi$ (**A**₈).

The following table summarizes the linear programming results.

(n, k)	$D_{LP}(n, k)$	$D(n, k)$	$Z_{LP}(n, k)$	$Z(n, k)$
$(4, 0)$	0.1362	0.1317	0	0
$(4, 1)$	0.208	0.20528	-0.0536	-0.05709
$(4, 2)$	0.3992	0.27886	-0.2	-0.11418
$(4, 3)$	0.6467	0.35244	-0.424	-0.17127
$(5, 0)$	0.3665	0.27113	-0.157	-0.05704
$(5, 1)$	0.5941	0.34471	-0.376	-0.11413
$(5, \geq 2)$	0.9706	$(4\pi\zeta - 8)pt$	*	*

The bound for $D(4, 0)$ comes from III.4.1.11. A few more comments are needed for $Z(4, 1)$. Let $S = S(y_1, \dots, y_6)$ be the anchored simplex that is not a quarter. If $y_4 \geq 2\sqrt{2}$ or $\text{dih}(S) \geq 2.2$, the linear programming bound is $< Z(4, 1)$. With this, if $y_1 \leq 2.75$, we have $\sigma(S) < Z(4, 1)$ by **A**₁₂. But if $y_1 \geq 2.75$, the 3 upright quarters along the upright diagonal satisfy

$$\nu < -0.3429 + 0.24573 \text{ dih}.$$

With this stronger inequality, the linear programming bound becomes $< Z(4, 1)$. This completes the proof of Theorem 4.4. \square

5.12 Some final estimates.

Recall that Section 4.4 defines an integer $n(R)$ that is equal to the number of sides if the region is a polygon. Recall that if the dihedral angle along an edge of a standard cluster is at most 1.32, then there is a flat quarter along that edge (Lemma 3.11.4).

Lemma 5.12.1. *Let R be an exceptional cluster with a dihedral angle ≤ 1.32 at a vertex v . Then R squanders $> t_n + 1.47 pt$, where $n = n(R)$.*

Proof. In most cases we establish the stronger bound $t_n + 1.5 pt$. In the proof of Theorem 4.4, we erase all upright diagonals, except those completely surrounded by anchored simplices. The contribution to t_n from the flat quarter Q at v in that proof is $D(3, 1)$ (Sections 4.5 and 5.5.1). Note that $\epsilon_\tau(Q) = 0$ here because there are no deformations. If we replace $D(3, 1)$ with $3.07 pt$ from Lemma 3.11.4, then we obtain the bound. Now suppose the upright diagonal is completely surrounded by anchored simplices. Analyzing the constants of Section 5.11, we see that $D_{LP}(n, k) - D(n, k) > 1.5 pt$, except when $(n, k) = (4, 1)$.

Here we have four anchored simplices around an upright diagonal. Three of them are quarters. We erase and take a penalty. Two possibilities arise. If the upright diagonal is enclosed over the flat quarter, its height is ≥ 2.6 by geometric considerations and the top face of the flat quarter has circumradius at least $\sqrt{2}$. The penalty is $2\xi'_\Gamma + \xi_V$, so the bound holds by the last statement of Lemma 3.11.4.

If, on the other hand, the upright diagonal is not enclosed over the flat diagonal, the penalty is $\xi_\Gamma + 2\xi_V$. In this case, we obtain the weaker bound $1.47 pt + t_n$:

$$3.07 pt > D(3, 1) + 1.47 pt + \xi_\Gamma + 2\xi_V.$$

\square

Remark. *If there are r nonadjacent vertices with dihedral angles ≤ 1.32 , we find that R squanders $t_n + r(1.47)$ pt .*

In fact, in the proof of the lemma, each $D(3, 1)$ is replaced with 3.07 pt from Lemma 3.11.4. The only questionable case occurs when two or more of the vertices are anchors of the same upright diagonal (a loop). Referring to Section 5.11, we have the following observations about various contexts.

- (4, 1) can mask only one flat quarter and it is treated in the lemma.
- (4, 2) can mask only one flat quarter and $D_{LP}(4, 2) - D(4, 2) > 1.47$ pt .
- (4, 3) cannot mask any flat quarters.
- (5, 0) can mask two flat quarters. Erase the five upright quarters, and take a penalty $4\xi_V + \xi_R$. We get

$$D(3, 2) + 2(3.07) \text{ pt} > t_5 + 4\xi_V + \xi_R + 2(1.47) \text{ pt}.$$

- (5, 1) can mask two flat quarters, and $D_{LP}(5, 1) - D(5, 1) > 2(1.47) \text{ pt}$.

Lemma 5.12.2. *Any pentagon with a dihedral angle less than 1.32 squanders at least 5.66 pt .*

Proof. To obtain the bound 5.66 pt , we argue as follows. If there are five anchored simplices surrounding a vertex, we have the bound by Table 5.11. If the configuration \mathbf{S}_4^+ or \mathbf{S}_3^- occurs, we squander at least $0.4 > 5.66$ pt (Sections 3.8 and 3.7). So if there are any upright diagonals in the pentagon that carry a penalty, we may assume they have four anchors. If there are no penalties, Lemma 3.11.4 gives $3.07 \text{ pt} + D(4, 1) > 5.66 \text{ pt}$. We do not need to deal with penalties from \mathbf{S}_3^+ in the score of the flat quarter at v because all penalties from a flat quarter are applied to the adjacent subregion (see Section 5.5 and Lemma 3.9.2). The only remaining possibility is four anchored simplices surrounding an upright diagonal. Unless there are three upright quarters, the bound follows from Section 5.11. If there are three upright quarters, erasing gives penalty $3\xi_R$, and $3.07 \text{ pt} + D(4, 1) - 3\xi_R > 5.66 \text{ pt}$. This proves the lemma for two pentagons and a quadrilateral. \square

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APPENDIX 1. INEQUALITIES

Let $\text{octavor}_0(Q) = 0.5(\text{vor}_0(Q) + \text{vor}_0(\hat{Q}))$, and $\text{octavor}(Q) = 0.5(\text{vor}(Q) + \text{vor}(\hat{Q}))$. We let τ_ν , τ_V , τ_0 , and τ_Γ be $-f + \text{sol}\zeta pt$, where $f = \nu$, vor , vor_0 , and Γ , respectively.

Each inequality is accompanied by one or more reference numbers. These identification numbers are needed to find further details about these calculations in [H1]. These inequalities were checked numerically before they were rigorously established, using a nonlinear optimization package. I thank the University of Maryland for this software.*

Edge lengths whose bounds are not specified are assumed to be between 2 and 2.51.

Most of the interval calculations in this appendix were completed by Samuel Ferguson. His calculations are marked with a dagger (\dagger).

Section A₁. β_ψ is defined in Section 2.8.

- 1: $\beta_\psi(y_1, y_3, y_5) < \text{dih}_3(S)$, if $y_2, y_3 \in [2, 2.23]$, $y_4 \in [2.77, 2\sqrt{2}]$, $\cos \psi = y_1/2.77$.
(We may assume $y_6 = 2$.) (757995764 \dagger)
- 2: $\beta_\psi(y_1, y_3, y_5) < \text{dih}_3(S)$, provided $y_4 = 3.2$, $y_5 = 2.51$, $y_6 = 2$, $\cos \psi = y_1/2.51$.
(735258244 \dagger)
- 3: $\beta_\psi(y_1, y_2, y_6) < \text{dih}_2(S)$, if $y_4 \in [2, 3.2]$, $y_5 = y_6 = 2.51$, $\psi = \text{arc}(y_1, t_0, 1.6)$.
(343330051 \dagger)
- 4: $\beta_\psi(y_1, y_2, y_6) < \text{dih}_2(S)$, if $y_4 \in [2, 3.2]$, $y_5 = 3.2$, $y_6 = 2$, $y_1 \in [2.2, 2.51]$,
 $\psi = \text{arc}(y_1, t_0, 1.6)$. (49446087 \dagger)
- 5: $\text{dih}(R(y_2/2, \eta_{126}, y_1/(2 \cos \psi))) < \text{dih}_2(S)$, if $y_1 \in [2, 2.2]$, $y_3 = 2.51$, $y_4 = 3.2$,
 $y_5 = 3.2$, $y_6 = 2$, $\psi = \text{arc}(y_1, t_0, 1.6)$. (799187442 \dagger)
- 6: $\text{vor}(Q, 1.385) < 0.00005$, if $y_4 \in [2.77, 2\sqrt{2}]$, and $\eta_{456} \geq \sqrt{2}$. (275706375)
- 7: $\text{vor}(Q, 1.385) < 0.00005$, if $y_4 \in [2.77, 2\sqrt{2}]$, and $\eta_{234} \geq \sqrt{2}$. (324536936)
- 8: $\tau_V(Q, 1.385) > 0.0682$, if $y_4 \in [2.77, 2\sqrt{2}]$, and $\eta_{456} \geq \sqrt{2}$. (983547118)
- 9: $\tau_V(Q, 1.385) > 0.0682$, if $y_4 \in [2.77, 2\sqrt{2}]$, and $\eta_{234} \geq \sqrt{2}$. (206278009)

Section A₂. In Inequalities A₂ and A₃, the domain is the set of upright quarters. The dihedral angle is measured along the diagonal.

- 1: $\nu < -4.3223 + 4.10113 \text{ dih}$. (413688580)
- 2: $\nu < -0.9871 + 0.80449 \text{ dih}$ (805296510)
- 3: $\nu < -0.8756 + 0.70186 \text{ dih}$ (136610219)
- 4: $\nu < -0.3404 + 0.24573 \text{ dih}$ (379204810)
- 5: $\nu < -0.0024 + 0.00154 \text{ dih}$ (878731435)
- 6: $\nu < 0.1196 - 0.07611 \text{ dih}$ (891740103)

Section A₃.

- 1: $-\tau_\nu < -4.42873 + 4.16523 \text{ dih}$ (334002329)
- 2: $-\tau_\nu < -1.01104 + 0.78701 \text{ dih}$ (883139937)
- 3: $-\tau_\nu < -0.99937 + 0.77627 \text{ dih}$ (507989176)
- 4: $-\tau_\nu < -0.34877 + 0.21916 \text{ dih}$ (244435805)
- 5: $-\tau_\nu < -0.11434 + 0.05107 \text{ dih}$ (930176500)
- 6: $-\tau_\nu < 0.07749 - 0.07106 \text{ dih}$ (815681339)

Section A₄.

– *Sphere Packings IV* – printed February 1, 2008

* www.isr.umd.edu/Labs/CACSE/FSQP/fsqp.html

In \mathbf{A}_4 and \mathbf{A}_5 , $y_1 \in [2.51, 2\sqrt{2}]$ and $y_4 \in [2.51, 2\sqrt{2}]$ and $\text{dih} < 2.46$. Let $\text{vor}_x = \text{vor}$ if the simplex is of type C and $\text{vor}_x = \text{vor}_0$ otherwise.

- 1: $\text{vor}_x < -3.421 + 2.28501 \text{ dih}$ (649592321)
- 2: $\text{vor}_x < -2.616 + 1.67382 \text{ dih}$ (600996944)
- 3: $\text{vor}_x < -1.4486 + 0.8285 \text{ dih}$ (70667639)
- 4: $\text{vor}_x < -0.79 + 0.390925 \text{ dih}$ (99182343)
- 5: $\text{vor}_x < -0.3088 + 0.12012 \text{ dih}$ (578762805)
- 6: $\text{vor}_x < -0.1558 + 0.0501 \text{ dih}$ (557125557)

Section \mathbf{A}_5 . Set $\tau_x = \text{sol } \zeta pt - \text{vor}_x$.

- 1: $-\tau_x < -3.3407 + 2.1747 \text{ dih}$ (719735900)
- 2: $-\tau_x < -2.945 + 1.87427 \text{ dih}$ (359616783)
- 3: $-\tau_x < -1.5035 + 0.83046 \text{ dih}$ (440833181)
- 4: $-\tau_x < -1.0009 + 0.48263 \text{ dih}$ (578578364)
- 5: $-\tau_x < -0.7787 + 0.34833 \text{ dih}$ (327398152)
- 6: $-\tau_x < -0.4475 + 0.1694 \text{ dih}$ (314861952)
- 7: $-\tau_x < -0.2568 + 0.0822 \text{ dih}$ (234753056)

Section \mathbf{A}_6 . In the Inequalities \mathbf{A}_6 and \mathbf{A}_7 , we assume $y_1 \in [2.51, 2\sqrt{2}]$, $y_4 \in [2\sqrt{2}, 3.2]$, and $\text{dih} < 2.46$.

- 1: $\text{vor}_0 < -3.58 + 2.28501 \text{ dih}$ (555481748)
- 2: $\text{vor}_0 < -2.715 + 1.67382 \text{ dih}$ (615152889)
- 3: $\text{vor}_0 < -1.517 + 0.8285 \text{ dih}$ (647971645)
- 4: $\text{vor}_0 < -0.858 + 0.390925 \text{ dih}$ (516606403)
- 5: $\text{vor}_0 < -0.358 + 0.12012 \text{ dih}$ (690552204)
- 6: $\text{vor}_0 < -0.186 + 0.0501 \text{ dih}$ (852763473)

Section \mathbf{A}_7 . The assumptions are as in \mathbf{A}_6 .

- 1: $-\tau_0 < -3.48 + 2.1747 \text{ dih}$ (679673664)
- 2: $-\tau_0 < -3.06 + 1.87427 \text{ dih}$ (926514235)
- 3: $-\tau_0 < -1.58 + 0.83046 \text{ dih}$ (459744700)
- 4: $-\tau_0 < -1.06 + 0.48263 \text{ dih}$ (79400832)
- 5: $-\tau_0 < -0.83 + 0.34833 \text{ dih}$ (277388353)
- 6: $-\tau_0 < -0.50 + 0.1694 \text{ dih}$ (839852751)
- 7: $-\tau_0 < -0.29 + 0.0822 \text{ dih}$ (787458652)

Section \mathbf{A}_8 . In all these except (125103581) and (504968542), the signs of all the partials except in the x_1 variable are easily determined by the methods of Section I.8. In this way, they become optimizations in one variable.

- 1: $\text{dih} > 1.23$ if $y_1 \in [2.51, 2\sqrt{2}]$, and $y_4 \geq 2.51$. (499014780)
- 2: $\text{dih} > 1.4167$, if $y_1 \in [2.51, 2\sqrt{2}]$, and $y_4 \geq 2\sqrt{2}$. (901845849)
- 3: $\text{dih} > 1.65$ if $y_1 \in [2.51, 2\sqrt{2}]$, $y_4 \geq 3.2$ (410091263)
- 4: $\text{dih} > 0.956$ if $y_1 \in [2.51, 2\sqrt{2}]$, $y_4 \geq 2$. (125103581)
- 5: $\text{dih} > 0.28$, if $y_1 \in [2.51, 2\sqrt{2}]$, $y_4 \geq 2$, $y_5 \in [2, 2\sqrt{2}]$. (504968542)
- 6: $\text{dih} > 1.714$, if $y_1 \in [2.7, 2\sqrt{2}]$, $y_4 \geq 3.2$ (770716154)
- 7: $\text{dih} > 1.714$, if $y_1 \in [2.51, 2.7]$, $y_4 \geq 3.2$, $y_2 \in [2, 2.25]$ (666090270)
- 8: $\text{dih} < 2.184$, if $y_1 \in [2.51, 2\sqrt{2}]$. (This one was simple enough to do without interval arithmetic.) (971555266)

Section \mathbf{A}_9^\dagger . $\kappa(S)$ is defined in Section 3.3.

- 1: $\kappa < -0.003521$, $y_1 \in [2.696, 2\sqrt{2}]$, $y_2, y_6 \in [2.45, 2.51]$, $y_4 \geq 2.77$, (956875054)

- 2: $\kappa < -0.017$, if $y_1 \in [2.51, 2.696]$, $y_4 \in [2.77, 2\sqrt{2}]$, $\eta_{234} \geq \sqrt{2}$. (664200787)
- 3: $\kappa < -0.017$, if $y_1 \in [2.51, 2.696]$, $y_4 \in [2.77, 2\sqrt{2}]$, $\eta_{456} \geq \sqrt{2}$. (390273147)
- 4: $\kappa < -0.02274 = \xi_{\kappa, \Gamma} - \xi'_\Gamma$, if $y_1 \in [2.57, 2\sqrt{2}]$, $y_4 \geq 3.2$, $\Delta \geq 0$. By monotonicity we may assume $y_4 = 3.2$. (654422246)
- 5: $\kappa < \xi_\kappa = -0.029$, if $y_1 \in [2.51, 2.57]$, $y_4 \geq 3.2$, $\Delta \geq 0$. By monotonicity we may assume $y_4 = 3.2$. (366536370)
- 6: $\kappa < -0.03883$, if $y_1 \in [2.51, 2.57]$, $y_2, y_3, y_5, y_6 \in [2, 2.25]$, $y_4 \geq 3.2$, $\Delta \geq 0$. By monotonicity we may assume $y_4 = 3.2$. (62532125)
- 7: $\kappa < -0.0325$, if $y_1 \in [2.51, 2.57]$, $y_2, y_3, y_5 \in [2, 2.25]$, $y_4 \geq 3.2$, $\Delta \geq 0$. By monotonicity we may assume $y_4 = 3.2$. (370631902)

Section A₁₀.

- 1: $\Gamma < \text{octavor}_0$, if $y_1 \in [2.696, 2\sqrt{2}]$. (214637273)
- 2: $\Gamma < \text{octavor}_0 + 0.01561$, if $y_1 \in [2.51, 2\sqrt{2}]$. (751772680)
- 3: $\Gamma < \text{octavor}_0 + 0.00935$, if $y_1 \in [2.57, 2\sqrt{2}]$. (366146051)
- 4: $\Gamma < \text{octavor}_0 + 0.00928$, if $y_1 \in [2.51, 2.57]$, $y_2 \in [2.25, 2.51]$. (675766140)
- 5: $\Gamma < \text{octavor}_0$, if $y_1 \in [2.51, 2.57]$, $y_2, y_6 \in [2.25, 2.51]$. (520734758)

Section A₁₁.

- 1: $\text{octavor} < \text{octavor}_0$, if $y_1 \in [2.696, 2\sqrt{2}]$, $y_2, y_3 \in [2, 2.45]$. (378432183)
- 2: $\text{octavor} < \text{octavor}_0$, if $y_1 \in [2.696, 2\sqrt{2}]$, $y_2, y_5 \in [2.45, 2.51]$. (572206659)
- 3: $\text{vor} < \text{vor}_0 + 0.003521$, if $y_1 \in [2.51, 2\sqrt{2}]$. (310679005)
- 4: $\text{vor} < \text{vor}_0 - 0.003521$, if $y_1 \in [2.696, 2\sqrt{2}]$, $y_2, y_6 \in [2.45, 2.51]$, $y_4 \in [2.51, 2.77]$. (284970880)
- 5: $\text{vor} < \text{vor}_0 - 0.009$, if $y_1 \in [2.51, 2.696]$, $y_4 \in [2.51, 2\sqrt{2}]$. (972111620)
- 6: $\text{octavor} < \text{octavor}_0$, if $y_1 \in [2.51, 2.57]$, $\eta_{126} \geq \sqrt{2}$. (875762896)
- 7: $\text{octavor} < \text{octavor}_0 - 0.004131$, if $y_1 \in [2.51, 2\sqrt{2}]$, $\eta_{126} \leq \sqrt{2}$, $\eta_{135} \geq \sqrt{2}$, $y_3 \leq 2.2$. (385332676)

Section A₁₂.

- 1: $\tau_V(S) > 0.13 + 0.2(\text{dih}(S) - \pi/2)$, if $y_1, y_2 \in [2.51, 2\sqrt{2}]$, and $\eta_{126}(S) \leq \sqrt{2}$. (970291025†)
- 2: $\tau_V(S, \sqrt{2}) > 0.13 + 0.2(\text{dih}(S) - \pi/2)$, if $y_1, y_2 \in [2.51, 2\sqrt{2}]$, and $\eta_{126}(S) \geq \sqrt{2}$. (524345535†)
- 3: $\nu < -0.3429 + 0.24573 \text{ dih}$, for upright quarters with $y_1 \in [2.75, 2\sqrt{2}]$. (812894433) ■
- 4: $\text{vor}_x < -0.0571$, for anchored simplices with $y_4 \in [2.51, 2\sqrt{2}]$, $y_1 \in [2.51, 2.75]$, $\text{dih} < 2.2$. (404793781)

Section A₁₃. Inequalities (74657942) and (675901554) hold by inspection. The others are verified in the usual manner.

- 1: $\tau_\nu(S) > 0.033$, if S is an upright quarter. (705592875)
- 2: $\tau_0(S) > 0.06585 - 0.0066$, if S is a flat quarter, and $y_4 = 2\sqrt{2}$. (747727191)
- 3: $\text{vor}_0(S) < 0.009$, if S is a flat quarter, and $y_4 = 2\sqrt{2}$. (474496219)
- 4: $\text{vor}_0(S(2, y_2, y_3, y_4, 2, 2)) < 0.0461$, if $y_4 \in [2\sqrt{2}, 3.2]$. (649551700)
- 5: $\text{vor}_0(S(2.51, 2, y_3, y_4, 2, 2)) \leq 0$, if $y_4 \in [2\sqrt{2}, 3.2]$. (74657942)
- 6: $\text{vor}_0(S(y_1, y_2, 2.51, y_4, 2, 2)) < 0$, if $y_4 \in [2\sqrt{2}, 3.2]$. (897129160)
- 7: $\tau_0(S(2, y_2, y_3, y_4, 2, 2)) > 0.014$, if $y_4 \in [2\sqrt{2}, 3.2]$. (760840103)
- 8: $\tau_0(S(2.51, 2, 2, y_4, 2, 2)) \geq 0$, if $y_4 \in [2\sqrt{2}, 3.2]$. (675901554)
- 9: $\tau_0(S(y_1, y_2, 2.51, y_4, 2, 2)) > 0.06585$, if $y_4 \in [2\sqrt{2}, 3.2]$. (712696695)
- 10: $\nu < \text{vor}_0 + 0.01(\pi/2 - \text{dih})$, if $y_1 \in [2.696, 2\sqrt{2}]$. (269048407)

- 11: $\nu < \text{vor}_0$, if $y_1 \in [2.6, 2.696]$, $y_4 \in [2.1, 2.51]$. (553285469)
- 12: $\mu < \text{vor}_0 + 0.0268$, if $y_4 \in [2.51, 2\sqrt{2}]$. (293389410)
- 13: $\mu < \text{vor}_0 + 0.02$, if $y_1 \in [2, 2.17]$, $y_4 \in [2.51, 2\sqrt{2}]$. (695069283)
- 14: $\text{dih} > 1.32$, if $y_4 = 2\sqrt{2}$. (814398901)
- 15: $\hat{\tau} > 3.07 \text{ pt}$, for all flat quarters satisfying $\text{dih} \leq 1.32$. (352079526)
- 16: $\tau_0 > 3.07 \text{ pt} + \xi_V + 2\xi'_\Gamma$, if $y_4 \in [2.51, 2\sqrt{2}]$, $\eta_{456} \geq \sqrt{2}$, $\text{dih} \leq 1.32$. (179025673)

Section \mathbf{A}_{14}^\dagger .

V_i is defined in Section 4.9. The function f is defined in Section 4.13.

- 1: $V_0 < 0$, if $\Delta \geq 0$, $y_4 \in [2, y_2 + y_3]$, $y_5 \in [2, 3.2]$, $y_6 \in [y_5, 3.2]$. (424011442)
- 2: $V_1 < 0$, if $\Delta \geq 0$, $y_4 \in [2, y_2 + y_3]$, $y_5 \in [2, 3.2]$, $y_6 \in [y_5, 3.2]$. (140881233)
- 3: $V_j + 0.82\sqrt{421} < 0$, if $y_5 \in [2, 2.189]$, $y_4 \in [2\sqrt{2}, 3.2]$, $y_6 \in [2, 2.51]$, $\Delta \geq 0$, $j = 0, 1$. (601456709)
- 4: $V_j + 0.82\sqrt{421} < 0$, if $y_5 \in [2, 2.189]$, $y_4 \in [3.2, y_2 + y_3]$, $y_6 \in [2, 3.2]$, $\Delta \geq 0$, $j = 0, 1$. (292977281)
- 5: $V_j + 0.5\sqrt{421} < 0$, if $y_5 \in [2.189, 2.51]$, $y_4 \in [2\sqrt{2}, 3.2]$, $y_5, y_6 \in [2, 2.51]$, $\Delta \geq 0$, $j = 0, 1$. (927286061)
- 6: $V_j + 0.5\sqrt{421} < 0$, if $y_5 \in [2.189, 3.2]$, $y_4 \in [3.2, y_2 + y_3]$, $y_5, y_6 \in [2, 3.2]$, $\Delta \geq 0$, $j = 0, 1$. (340409511)
- 7: $\Delta < 421$, if $y_4 \in [2\sqrt{2}, y_2 + y_3]$, $y_5, y_6 \in [2, 3.2]$, $\eta(x_1, x_3, x_5) \leq t_0$. (727498658)
- 8: $-4\delta_{\text{oct}}u_{135}\partial/\partial x_5(\text{quo}(R_{135}) + \text{quo}(R_{315})) < 0.82$. (484314425)
- 9: $-4\delta_{\text{oct}}u_{135}\partial/\partial x_5(\text{quo}(R_{135}) + \text{quo}(R_{315})) < 0.5$, if $y_5 \in [2.189, 2.51]$. (440223030)
- 10: $f(y_1, y_2) \geq 0.887$, $\lambda = 1.945$, $y_1, y_2 \in [2, 2.51]$. (115756648)

Section \mathbf{A}_{15}^\dagger . Let $D^i f_j = \partial^i f_j(S)/\partial x_1^i$, $f_0 = \text{vor}_0$, $f_1 = -\tau_0$, as in Section 5.1.

- 1: $D^2 f_i > 0$ if $Df_i = 0$, if $\Delta \geq 0$, $y_4 \geq 2\sqrt{2}$, $y_5 = 2$, $y_6 = 2$, $y_4 \leq y_2 + y_3$, $y_5 + y_6$, $i = 0, 1$. (329882546)
- 2: $D^2 f_i > 0$ if $Df_i = 0$, if $\Delta \geq 0$, $y_4 \geq 2\sqrt{2}$, $y_5 = 2$, $y_6 = 2.51$, $y_4 \leq y_2 + y_3$, $y_5 + y_6$, $i = 0, 1$. (427688691)
- 3: $D^2 f_i > 0$ if $Df_i = 0$, if $\Delta \geq 0$, $y_4 \geq 2\sqrt{2}$, $y_5 = 2$, $y_6 = 2\sqrt{2}$, $y_4 \leq y_2 + y_3$, $y_5 + y_6$, $i = 0, 1$. (562103670)
- 4: $D^2 f_i > 0$ if $Df_i = 0$, if $\Delta \geq 0$, $y_4 \geq 2\sqrt{2}$, $y_5 = 2.51$, $y_6 = 2.51$, $y_4 \leq y_2 + y_3$, $y_5 + y_6$, $i = 0, 1$. (564506426)
- 5: $D^2 f_i > 0$ if $Df_i = 0$, if $\Delta \geq 0$, $y_4 \geq 2\sqrt{2}$, $y_5 = 2.51$, $y_6 = 2\sqrt{2}$, $y_4 \leq y_2 + y_3$, $y_5 + y_6$, $i = 0, 1$. (288224597)
- 6: $D^2 f_i > 0$ if $Df_i = 0$, $\Delta \geq 0$, $y_4 \geq 2\sqrt{2}$, $y_5 = 2\sqrt{2}$, $y_6 = 2\sqrt{2}$, $y_4 \leq y_2 + y_3$, $y_5 + y_6$, $i = 0, 1$. (979916330, 749968927)

Section \mathbf{A}_{16} . Recall $D(3, 2) = 0.13943$, $Z(3, 2) = -0.05714$, $D(3, 1) = 0.06585$. Some of these follow from known results. See II.4.5.1, F.3.13.1, F.3.13.3, F.3.13.4. The case $\text{vor} \leq 0$ of the inequality $\sigma \leq 0$ for flat quarters follows by Rogers's monotonicity lemma I.8.6.2 and F.3.13.1, because the circumradius of the flat quarter is at least $\sqrt{2}$ when the analytic Voronoi function is used. We also use that $\text{vor}(R(1, \eta(2, 2, 2)\sqrt{2})) = 0$.

- 1: $\tilde{\tau}(S) > 0.06585$, if S is a flat quarter and $\tilde{\tau}(S)$ is any of the functions for flat quarters in Section 3.10, other than $\tau(S, 1.385)$, which is treated in \mathbf{A}_1 . (695180203)
- 2: $\tilde{\sigma}(S) \leq 0$, if S is a flat quarter and $\tilde{\sigma}(S)$ is any of the functions for flat quarters in Section 3.10, other than $\text{vor}(S, 1.385)$, which is treated in \mathbf{A}_1 . (690626704)
- 3: $\text{vor}(S) < Z(3, 2)$, for simplices S of type S_A . (807023313)
- 4: $\tau_V(S) > 0.13943$, for simplices S of type S_A . (590577214)

- 5: $\text{vor}_0(S) < Z(3, 2)$, if $y_4, y_5 \in [2.51, 2\sqrt{2}]$, and the simplex S is not of type S_A .
(949210508)
- 6: $\tau_0(S) > 0.13943$, if $y_4, y_5 \in [2.51, 2\sqrt{2}]$, and the simplex S is not of type S_A .
(671961774)

Section \mathbf{A}_{17}^\dagger . Let $y_4, y_5, y_6 \in [2, 3.2]$. Let k_0, k_1, k_2 be the number of variables in $[2, 2.51]$, $[2.51, 2\sqrt{2}]$, $[2\sqrt{2}, 3.2]$, respectively. (Make the intervals disjoint so that $k_0 + k_1 + k_2 = 3$.) Assume $k_1 + 2k_2 > 2$. ($k_1 + 2k_2 = 2$ gives special simplices or cases treated in \mathbf{A}_{16} .) We have $3\xi_\Gamma = 0.04683$.

Set

$$\pi'_\tau = \begin{cases} 0, & k_2 = 0, \\ 0.0254, & k_0 = k_1 = k_2 = 1, \\ 0.04683 + (k_0 + 2k_2 - 3)0.008/3 + k_2(0.0066), & \text{otherwise.} \end{cases}$$

- 1: $\tau_0(S) - \pi'_\tau > D(3, k_1 + k_2)$, for parameters (k_0, k_1, k_2) satisfying $k_0 + k_1 + k_2 = 3$, $k_1 + 2k_2 > 2$. (645264496)
- 2: $\tau_0(S) - 0.034052 > D(3, 2)$, if $y_4 \in [2.6, 2\sqrt{2}]$, $y_5 \in [2\sqrt{2}, 3.2]$. (910154674)
- 3: $\tau_0(S) - (0.034052 + 0.0066) > D(3, 2)$, if $y_6 = 2, y_4 = 2.51, y_5 = 3.2$. (877743345)

Section \mathbf{A}_{18}^\dagger . In the same context as \mathbf{A}_{17} , set

$$\pi'_\sigma = \begin{cases} 0, & k_2 = 0, \\ 0.009, & k_0 = 0, k_2 = 1, \\ (k_0 + 2k_2)0.008/3 + 0.009k_2, & \text{otherwise.} \end{cases}$$

- 1: $\text{vor}_0(S) + \pi'_\sigma < Z(3, k_1 + k_2)$, for parameters (k_0, k_1, k_2) as above. (612259047)

Section \mathbf{A}_{19}^\dagger . Let Q be a quadrilateral subcluster whose edges are described by the vector

$$(a_1, 2, 2, 2, 2, 2, a_4, b_4).$$

Assume both diagonals have lengths in $[2\sqrt{2}, 3.2]$.

$$\begin{aligned} \tau_0(Q) &> 0.235 \quad \text{and} \quad \text{vor}_0(Q) < -0.075, \text{ if } b_4 \in [2.51, 2\sqrt{2}], \\ \tau_0(Q) &> 0.3109 \quad \text{and} \quad \text{vor}_0(Q) < -0.137, \text{ if } b_4 \in [2\sqrt{2}, 3.2], \end{aligned}$$

(357477295)

Section \mathbf{A}_{20}^\dagger . Let Q be a quadrilateral subcluster whose edges are described by the vector

$$(2, 2, a_2, 2, 2, b_3, a_4, b_4).$$

Assume $b_4 \geq b_3$, $b_4 \in \{2.51, 2\sqrt{2}\}$, $b_3 \in \{2, 2.51, 2\sqrt{2}\}$, $a_2, a_4 \in \{2, 2.51\}$. Assume that the diagonal between corners 1 and 3 has length in $[2\sqrt{2}, 3.2]$, and that the other diagonal has length ≥ 3.2 . Let k_0, k_1, k_2 be the number of b_i equal to 2, 2.51, $2\sqrt{2}$, respectively. If $b_4 = 2.51$ and $b_3 = 2$, no such subcluster exists (the reader can check that $\Delta(4, 4, x_3, 4, 2.51^2, x_6) < 0$ under these conditions), and we exclude this case.

- 1: $\text{vor}_0(Q) < Z(4, k_1 + k_2) - 0.009k_2 - (k_0 + 2k_2)0.008/3$. (193776341)
- 2: $\tau_0(Q) > D(4, k_1 + k_2) + 0.04683 + (k_0 + 2k_2 - 3)0.008/3 + 0.0066k_2$. (898647773)

- 3: $\text{vor}_0(Q) < Z(4, 2) - 0.0461 - 0.009 - 2(0.008)$, if $a_2 \in \{2, 2.51\}$, $a_4 = 2$, $b_4 = 2\sqrt{2}$,
 $b_3 = 2.51$ or $2\sqrt{2}$. (844634710)
- 4: $\tau_0(Q) > D(5, 1) + 0.04683 + 0.008 + 2(0.0066)$, if $a_2 \in \{2, 2.51\}$, $a_4 = 2$, $b_4 = 2\sqrt{2}$,
 $b_3 = 2.51$ or $2\sqrt{2}$. (328845176)
- 5: $\text{vor}_0(Q) < s_5 - 0.0461 - 0.008$, if $a_2 \in \{2, 2.51\}$, $a_4 = 2$, $b_3 = 2$, $b_4 = 2\sqrt{2}$.
(233273785)
- 6: $\tau_0(Q) > t_5 + 0.008$, if $a_2 \in \{2, 2.51\}$, $a_4 = 2$, $b_3 = 2$, $b_4 = 2\sqrt{2}$. (966955550)
- (The penalties used in \mathbf{A}_{20} are from Sections 5.4 and 5.5.)

Section \mathbf{A}_{21}^\dagger . Recall that $\pi_{\max} = 0.06688$.

- 1: $\text{vor}_0(S(2, 2, 2, y_4, 2, 2)) + \text{vor}_0(S(2, 2, 2, y'_4, 2, 2)) + \text{vor}_0(S(2, 2, 2, y_4, y'_4, 2)) < s_5 -$
 0.008 , if $y_4, y'_4 \in [2\sqrt{2}, 3.2]$. (275286804)
- 2: $\tau_0(S(2, 2, 2, y_4, 2, 2)) + \tau_0(S(2, 2, 2, y'_4, 2, 2)) + \tau_0(S(2, 2, 2, y_4, y'_4, 2)) > t_5 + 0.008$,
if $y_4, y'_4 \in [2\sqrt{2}, 3.2]$. (627654828)
- 3: $\text{vor}_0(S(2, 2, 2, y_4, y_5, y_6)) < -2(0.008) + s_6 - 3(0.0461)$, if $y_4, y_5, y_6 \in [2\sqrt{2}, 3.2]$.
(Compare \mathbf{A}_{13} .) (995177961)
- 4: $\tau_0(S(2, 2, 2, y_4, y_5, y_6)) > t_6 + \pi_{\max}$, if $y_4, y_5, y_6 \in [2\sqrt{2}, 3.2]$. (735892048)

Section \mathbf{A}_{22}^\dagger . In \mathbf{A}_{22} and \mathbf{A}_{23} , $y_1 \in [2.51, 2\sqrt{2}]$, $y_4 \in [2\sqrt{2}, 3.2]$, and $\text{dih} < 2.46$.
 $\text{vor}_0(Q)$ denotes the truncated Voronoi function on the union of an anchored simplex
and an adjacent special simplex. Let S' be the special simplex. By deformations,
 $y_1(S') \in \{2, 2.51\}$. If $y_1(S') = 2.51$, the verifications follow from \mathbf{A}_6 and $\text{vor}_0(S') \leq$
 0 . We may assume that $y_1(S') = 2$. Also by deformations, $y_5(S') = y_6(S') = 2$.

- 1: $\text{vor}_0(Q) < -3.58 + 2.28501 \text{ dih}$ (53502142)
- 2: $\text{vor}_0(Q) < -2.715 + 1.67382 \text{ dih}$ (134398524)
- 3: $\text{vor}_0(Q) < -1.517 + 0.8285 \text{ dih}$ (371491817)
- 4: $\text{vor}_0(Q) < -0.858 + 0.390925 \text{ dih}$ (832922998)
- 5: $\text{vor}_0(Q) < -0.358 + 0.009 + 0.12012 \text{ dih}$ (724796759)
- 6: $\text{vor}_0(Q) < -0.186 + 0.009 + 0.0501 \text{ dih}$ (431940343)

When the cross-diagonal drops to 2.51. We break Q into two simplices in the
other direction. Let S'' be an upright quarter with $y_5 = 2.51$. In the next group
 $\text{vor}_0 = \text{vor}_0(S'')$

- 7: $\text{vor}_0 < -3.58/2 + 2.28501 \text{ dih}$ (980721294)
- 8: $\text{vor}_0 < -2.715/2 + 1.67382 \text{ dih}$ (989564937)
- 9: $\text{vor}_0 < -1.517/2 + 0.8285 \text{ dih}$ (263355808)
- 10: $\text{vor}_0 < -0.858/2 + 0.390925 \text{ dih}$ (445132132)
- 11: $\text{vor}_0 < (-0.358 + 0.009)/2 + 0.12012 \text{ dih} + 0.2(\text{dih} - 1.23)$ (806767374)
- 12: $\text{vor}_0 < (-0.186 + 0.009)/2 + 0.0501 \text{ dih} + 0.2(\text{dih} - 1.23)$ (511038592)

Section \mathbf{A}_{23}^\dagger . $\tau_0(Q)$ denotes the truncated Voronoi function on the union of an
anchored simplex (with $y_1 \in [2.51, 2\sqrt{2}]$, $y_4 \in [2\sqrt{2}, 3.2]$, $\text{dih} < 2.46$) and an adja-
cent special simplex.

- 1: $-\tau_0(Q) + 0.06585 < -3.48 + 2.1747 \text{ dih}$ (4591018)
- 2: $-\tau_0(Q) + 0.06585 < -3.06 + 1.87427 \text{ dih}$ (193728878)
- 3: $-\tau_0(Q) + 0.06585 < -1.58 + 0.83046 \text{ dih}$ (2724096)
- 4: $-\tau_0(Q) + 0.06585 < -1.06 + 0.48263 \text{ dih}$ (213514168)
- 5: $-\tau_0(Q) + 0.06585 < -0.83 + 0.34833 \text{ dih}$ (750768322)
- 6: $-\tau_0(Q) + 0.06585 < -0.50 + 0.1694 \text{ dih}$ (371464244)
- 7: $-\tau_0(Q) + 0.06585 < -0.29 + 0.0014 + 0.0822 \text{ dih}$ (657011065)

Let S' be the special simplex. By deformations, we have $y_5(S') = y_6(S') = 2$, and

$y_1(S') \in \{2, 2.51\}$. If $y_1(S') = 2.51$, and $y_4(S') \leq 3$, the inequalities listed above follow from Section **A**₇ and the inequality

$$8: \tau_0(S') > 0.06585, \text{ if } y_1 = 2.51, y_4 \in [2\sqrt{2}, 3], y_5 = y_6 = 2. \quad (66753311)$$

Similarly, the result follows if y_2 or $y_3 \geq 2.2$ from the inequality

$$9: \tau_0(S') > 0.06585, \text{ if } y_4 \in [3, 3.2], y_5 = y_6 = 2, y_1 = 2.51, y_2 \in [2.2, 2.51]. \quad (762922223)$$

Because of these reductions, we may assume in the first batch of inequalities of **A**₂₃ that when $y_1(S') \neq 2$, we have that $y_1(S') = 2.51, y_5(S') = y_6(S') = 2, y_4 \in [3, 3.2], y_2(S'), y_3(S') \leq 2.2$. In all but (371464244) and (657011065), if $y_1(S') = 2.51$, we prove the inequality with $\tau_0(S')$ replaced with its lower bound 0.

Again if the cross-diagonal is 2.51, we break Q in the other direction. Let S'' be an upright quarter with $y_5 = 2.51$. Set $\tau_0 = \tau_0(S'')$. We have

$$10: -\tau_0 + 0.06585/2 < -3.48/2 + 2.1747 \text{ di}h \quad (953023504)$$

$$11: -\tau_0 + 0.06585/2 < -3.06/2 + 1.87427 \text{ di}h \quad (887276655)$$

$$12: -\tau_0 + 0.06585/2 < -1.58/2 + 0.83046 \text{ di}h \quad (246315515)$$

$$13: -\tau_0 + 0.06585/2 < -1.06/2 + 0.48263 \text{ di}h \quad (784421604)$$

$$14: -\tau_0 + 0.06585/2 < -0.83/2 + 0.34833 \text{ di}h \quad (258632246)$$

$$15: -\tau_0 + 0.06585/2 < -0.50/2 + 0.1694 \text{ di}h + 0.03(\text{di}h - 1.23) \quad (404164527)$$

$$16: -\tau_0 + 0.06585/2 < -0.29/2 + 0.0014/2 + 0.0822 \text{ di}h + 0.2(\text{di}h - 1.23) \quad (163088471) \blacksquare$$

Section A₂₄[†]. These final calculations here are used to determine what is squandered when $\text{di}h > 2.46$.

$$1: \tau_0 + 0.0822 \text{ di}h > 0.159, \text{ if } y_1 \in [2.51, 2\sqrt{2}], y_6 \in [2.51, 2.75], y_2 = y_4 = 2. \quad (968721007)$$

$$2: \text{di}h < 1.23 \text{ if } y_1 \in [2.51, 2\sqrt{2}], y_6 \geq 2.51, y_2 = 2.51, y_4 = 2. \quad (783968228)$$

$$3: \text{di}h < 1.23 \text{ if } y_1 \in [2.51, 2\sqrt{2}], y_6 \geq 2.75, y_2 = y_4 = 2. \quad (745174731)$$

APPENDIX 2. SOME CONVENTIONS

Throughout the paper, we have preferred to work with compact domains. As we divide cases into compact sets, boundaries will overlap. This leads to various mild inconsistencies unless certain statements in the paper are interpreted appropriately.

For example, if an edge of a quasi-regular tetrahedron is exactly 2.51, the quasi-regular tetrahedron is also a quarter. If some of the simplices along that edge are interpreted as quasi-regular tetrahedra and others are interpreted as quarters, this could easily have unintended effects. In such cases we ask the reader to decide once and for all whether the edge is to be considered the diagonal of a quarter or as a short edge of a quasi-regular tetrahedron, and then adhere to that convention.

In general when a length lies on the boundary between two cases, the inequalities have been designed to hold for whichever of the two cases is selected, as long as the selection is consistently adhered to.

When we divide the domain into several compact regions, and divide a function piecewise on each region, in several places we use an abbreviated style that might create ambiguities for function values at boundary cases. Again we ask the reader to adhere to any consistent convention.

In most cases, bounds on the score are strict. There are only a few places where exact equality can be obtained and where it makes an appreciable difference. The most significant are the bounds $\sigma \leq pt$ on quasi-regular tetrahedra and $\sigma \leq 0$ on quad-clusters. The fact that these are attained for the regular cases with edge lengths 2 and diagonal $2\sqrt{2}$ on the quad-cluster and for no other cases gives the bound $\pi/\sqrt{18}$ on density and the local optimality of the fcc and hcp packings.

Another place where we have allowed equality to be obtained is with $\tau_0 \geq 0$ for quasi-regular simplices. The importance of equality for Rogers's bound on the density of packings is explained in III.

There are also a few less significant cases where an inequality is sharp. For example,

$$\tau_0(2.51, 2, 2, x, 2, 2) \geq 0, \quad \text{vor}_0(2.51, 2, 2, x, 2, 2) \leq 0$$

for special simplices satisfying $x \in [2\sqrt{2}, 3.2]$. Also, equality occurs in Lemma F.1.9 and F.2.2.